HIGH-END COMPUTING CAPABILITY PORTFOLIO

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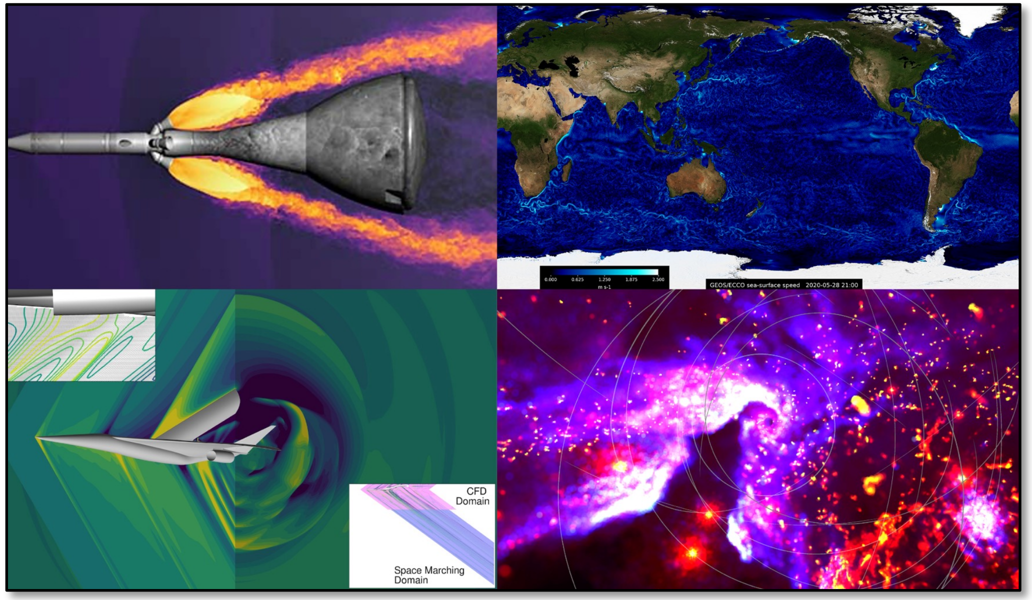
National Aeronautics and Space Administration

New Allocation Period for Supercomputer Time Begins for NASA Mission Directorates

- The new allocation period for all NASA mission directorates began October 1, 2022.
  - Mission directorates allocated approximately 271.5 million Standard Billing Units (SBUs) to 718 projects.
  - The Aeronautics Mission Directorate allocated just under 61.5 million SBUs to 146 projects.
  - The Exploration Systems Development, Space Operations, and Space Technology mission directorates, and NASA Engineering and Safety Center collectively allocated more than 48 million SBUs to 74 projects.
  - The Science Mission Directorate allocated more than 98 million SBUs to 452 projects.
- Continuing Human Exploration and Operations Mission Directorate projects were mapped to the current mission, program, and project. Sponsoring programs and projects were also updated for the Space Technology Mission Directorate to improve reporting.
- The Request Management System (RMS) ensured a smooth process for principal investigators, allocators, and HECC staff.
  - Provides easy navigation to create requests, adjust SBUs, extend project end dates, cancel, and print request PDFs.
  - Added Commercial Cloud to the intake form.

IMPACT: NASA programs and projects periodically review the distribution of supercomputer time to assess demand for resources and assure consistency with mission-specific goals and objectives.

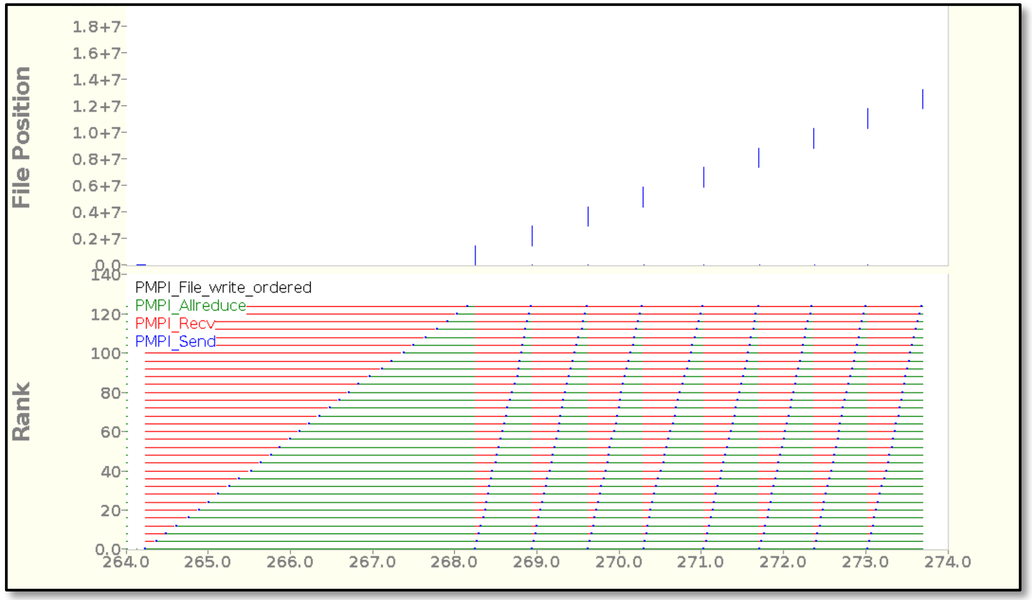


Clockwise from left: Simulation of the AA-2 launch abort vehicle; Sea-surface speed, in a snapshot from a coupled ocean-atmosphere simulation; screenshot of the Galactic Center virtual reality app; Pressure wave radiating from the LM 1044 low-boom wind tunnel model.

APP Experts Improve I/O Performance of StellarBox Code

- HECC's Applications Performance and Productivity (APP) team improved the I/O performance of the StellarBox code by 22x, which resulted in about a 6x speedup in overall runtime on the Aitken Rome nodes.
  - StellarBox is used for 3D simulations of radiative magnetohydrodynamic processes on the Sun or stars; it is one of the top five applications in standard billing units (SBUs) consumption for HECC in FY22.
- The APP team identified the I/O bottlenecks and developed solutions using a small test case. The solutions were successfully demonstrated and implemented on production cases.
  - One bottleneck came from the first phase of the collective calls to the function *MPI_File_write_ordered*, which is serialized in nature. Reducing the total number of MPI ranks of the run decreased the time spent there.
  - The second bottleneck was due to competition for physical core resources among the processes of the application and other tasks running on the system when hyperthreading (HT) is disabled. Enabling HT or simply cutting the number of MPI ranks per node by half and spreading the ranks between the two sockets of a Rome node eliminated this contention.
- StellarBox users in the NAS Division have started using the solutions and are excited about the improvements. The APP team continues to investigate other solutions for additional performance gains.

IMPACT: Improving the performance of heavily used codes such as StellarBox allows for more efficient use of HECC's newest resources, which are in high demand among users.

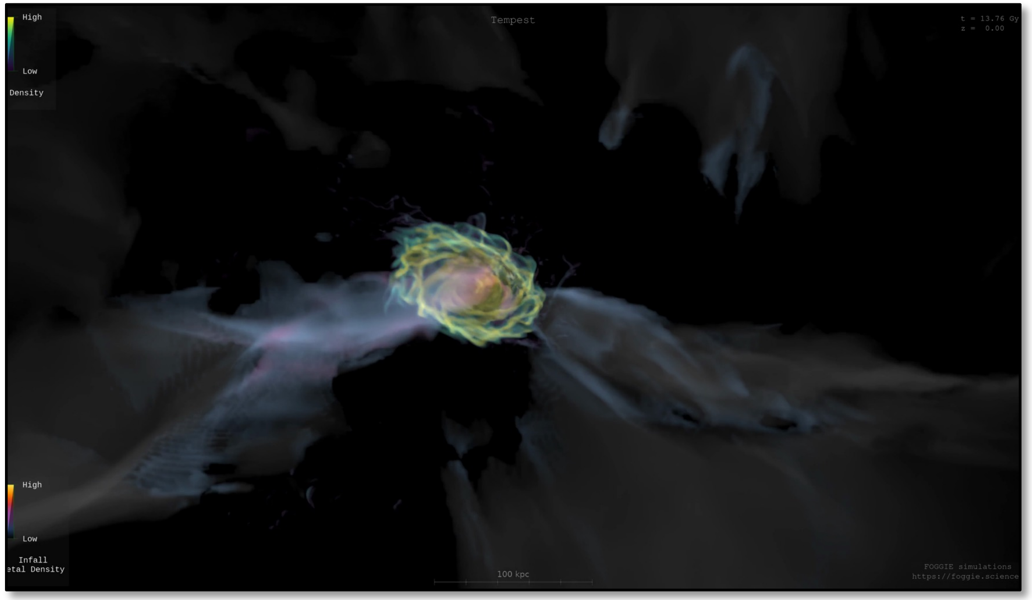


The serialized communication phase (bottom panel) and the POSIX I/O phase (top panel) of the *MPI_File_write_ordered* calls against time (x-axis), as illustrated through the IOT tool for a StellarBox run on the Aitken Rome nodes.

Visualization Team Adds Conditional Rendering Capability for Data Exploration

- HECC visualization experts enhanced their production codebase to support a style of conditional rendering used in exploratory data analysis.
  - Although limited in the initial implementation, this work could support a wide range of renderings where information from two fields can be used at once during rendering.
  - For example, the enhanced codebase could provide coloring by “Metal Density” and show it only where the infall velocity is above a threshold.
- Enhancements added to Intel’s open-source OSPRay ray tracing engine allow volume rendering where color is taken from one scalar and transparency is taken from another.
  - Examination of the OSPRay code suggested some relatively simple modifications that would allow using two fields at once to set color and opacity when rendering volumes.
  - These modifications were added to the latest version of OSPRay, v2.10.0. Code was also added to an HECC production renderer to take advantage of these changes, and animations were generated using recent data from the researcher.
- Further enhancements could generalize to full conditional queries, such as: “show me the data where A and B are true.”

IMPACT: This HECC visualization work supports conditional rendering, a powerful capability that provides researchers the ability to explore questions like: “show me the metallicity where the velocity is high.”

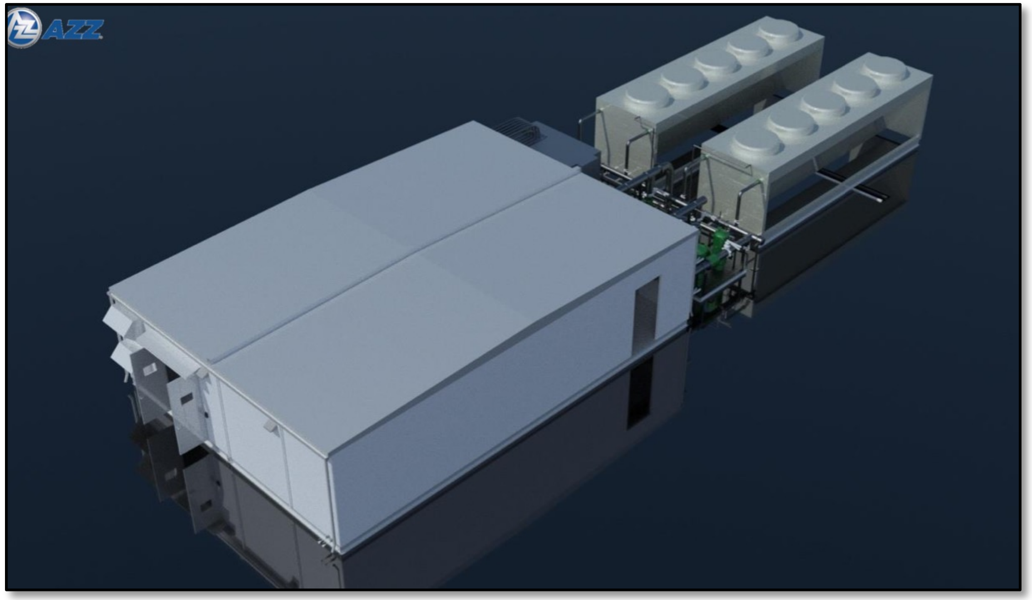


Metal-rich material falling into a galactic disk. *Cassi Lochhaas, Space Telescope Science Institute; Tim Sandstrom, NASA/Ames*

Modular Supercomputing Facility Expansion Begins

- On October 21, 2022, HECC awarded a contract to AZZ Inc. of Millington, Maryland, to produce the second Aitken compute module at the Modular Supercomputing Facility (MSF) at NASA Ames.
- AZZ will supply the prefabricated metal building along with the electrical and cooling infrastructure to support expansion of the Aitken supercomputer.
- Compute Module 2 (CM2) will have 3 megawatts (MW) of electrical computing capacity, bringing the power available for Aitken computing operations to 5 MW.
- The Aitken expansion into CM2 will begin with HPE Apollo Racks powered by AMD Milan processors. CM2 and the Aitken expansion are expected to be in operation in early 2024. (Worldwide supply chain issues are affecting equipment lead times.)
- The MSF is capable of housing up to 12 compute modules and up to 3 data storage modules in future expansions.

IMPACT: The expansion of the Modular Supercomputing Facility with a second module will double the size of the Aitken supercomputer, providing substantially more computing resources for the HECC user community.

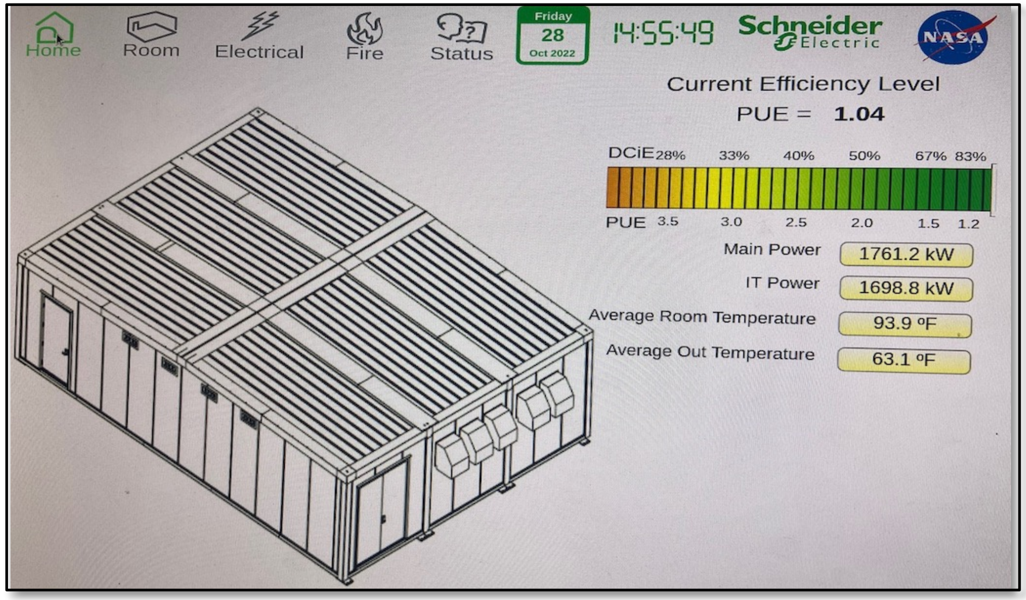


A graphical rendering of Compute Module 2 and its support infrastructure, to be installed at the Modular Supercomputing Facility at NASA Ames. *AZZ Inc & Avail Infrastructure Solutions*

HECC Systems Reach New Power Usage Peak

- HECC's Pleiades, Electra, and Aitken supercomputers, and data storage systems recorded their highest combined average power usage at 6.8 megawatts (MW) for the quarterly period July through September 2022. The latest Aitken expansion and uptime improvements drove the power usage peak.
- The combined facility power (for N258, R&D088, and R&D099) also recorded a highest average power at 8.3MW for the quarter.
- The overall supercomputing Power Usage Effectiveness (PUE) for the period was 1.22; Aitken and Electra each came in at 1.05 PUE.
  - PUE, an established metric for computer center power efficiency, is calculated as the (Total Facility Power) ÷ (IT Systems Power).
  - In comparison, the reported average PUE for data centers around the world is 1.8; and the PUE for all of NASA is 1.48.
- With rising energy costs, low-PUE facilities are more important than ever. Operating Electra and Aitken in the low-PUE modules of R&D088 and R&D099 saves over $1 million per year in energy costs, when compared to the N258 traditional data center.

IMPACT: The energy savings provided by HECC's low Power Usage Effectiveness facilities allow for more HECC funds to be spent on computing and storage resources.



The Building Management Software control screen for the R&D099 facility housing the Aitken Supercomputer, as shown operating with a 1.04 PUE. *Chris Tanner, NASA.*

RMS Team Holds Successful Planning Workshop

- The Request Management System (RMS) team held a three-day hybrid workshop focused on backlog grooming, release planning, and establishing priority levels and level of effort for development. Of the 187 tasks evaluated:
  - 22 were removed as duplicates or resolved by other version enhancements.
  - 57 were rated as high priority, with complexity ranging from very difficult to low/simple change.
  - 20 stories were rated as medium priority.
  - 36 stories were rated low or lowest in terms of priority, with varying levels of complexity. These are the most likely to be evaluated in the next workshop to see if they are still required.
- The RMS team employed the Fibonacci Scale to organize versions:
  - The project revolves around units of work called 'stories' in an Agile project management.
  - Each version is limited to 20 story points. Story points represent the size, complexity, and effort needed to complete a user story.
  - Each story in the backlog was reviewed for priority and level of complexity as well as which logical grouping they belong in, such as Cloud, Infrastructure, or User Interface.
  - Each version is made up of varying levels of complexity totaling approximately 20 Fibonacci Scale points.
  - Using these logical groupings and complexity levels, the team created version release planning over the next three months in detail, and wide-ranging plans for the next six months based on priority needs.
- The RMS team is planning a second workshop for release planning, to be hosted at NASA Goddard in April 2023.

IMPACT: The workshop enabled advanced planning for short- and long-term version releases by providing priority and level of effort involved for development.

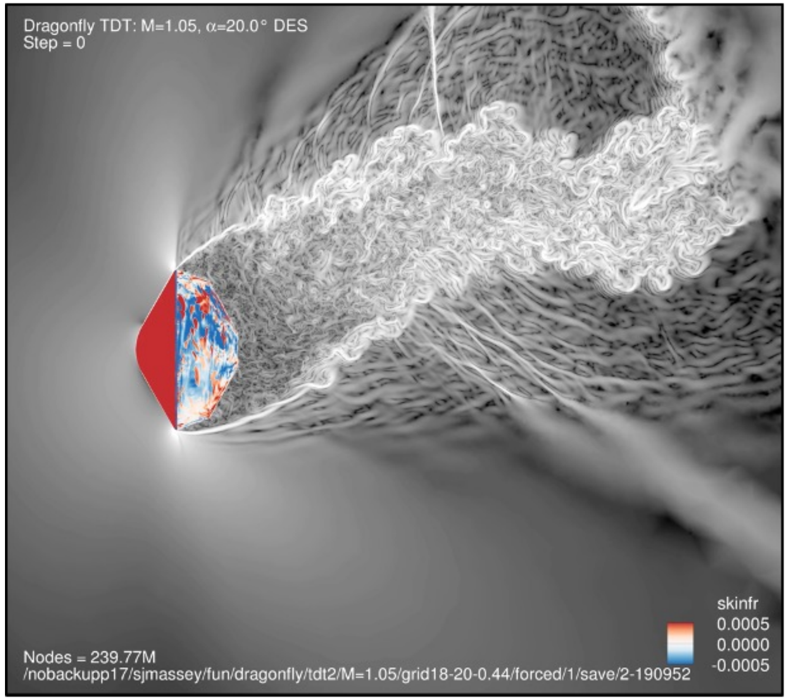
The Whirlpool Galaxy is a classic Fibonacci spiral galaxy. This image is a digital combination of a ground-based image from the 0.9-meter telescope at Kitt Peak National Observatory and a space-based image from the Hubble Space Telescope, highlighting sharp features normally too red to be seen. *NASA/Hubble*

HECC GPUs Accelerate Dynamic Stability Derivatives for Dragonfly*

- Aerospace engineers at NASA Langley (LaRC) are conducting computational fluid dynamics (CFD) simulations to predict the capsule dynamic pitch stability derivatives at low supersonic and transonic speeds for the agency's Dragonfly mission. This mission will fly multiple sorties to sample and examine sites around Saturn's moon, Titan.
- The team's transonic forced oscillation CFD analyses, obtained using the FUN3D CFD tool, augment testing in the LaRC Transonic Dynamics Tunnel, a unique wind tunnel facility that is optimized for aeroelastic, dynamic, or high-risk testing.
- Statistically-converged values of pitch damping coefficient require at least 10 oscillation cycles to be run on HECC supercomputers. Wall clock time on the finest grid (240 million grid points):
  - 48 Rome CPU nodes: 117.5 hours per cycle, or 7 weeks for 10 cycles.
  - 28 4xV100 GPU nodes: 19.8 hours per cycle, or 8 days for 10 cycles.
- Dragonfly will launch in 2026 and arrive in 2034, looking for signs of life on Titan, and can provide clues to how life may have arisen on our planet.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: Graphics processing units (GPUs) on HECC's Pleiades supercomputer are being used to substantially reduce turnaround time for long-duration simulations required to converge statistical quantities such as pitch-rate derivatives.



Surface contours of skin friction and density gradients on a mid-span slice of the flow field for the Dragonfly rotorcraft-lander.
Steve Massey, NASA Langley

Convection in High-Resolution Global Solar Simulations*

- Researchers at the New Jersey Institute of Technology and NASA Ames Research Center worked together to use 3D global models of the Sun to help improve the understanding of the driving mechanisms within the convection zone of the solar interior.
- The convection zone of the Sun consists of the upper 30% of the solar interior and is characterized by jets of rising and falling plasma driven by the heat generated in the core. These jets, along with solar rotation, are responsible for most solar activity, including differential rotation and meridional circulation, which ultimately drive the solar dynamo and generate the Sun's magnetic field.
- The team used the 3D global hydrodynamic code EULAG to simulate the convective action of plasma throws throughout the solar interior. Their simulations exhibited similar patterns of multiscale convection generated by a solar-like density stratification, as seen in high-resolution observations made by NASA's Solar Dynamics Observatory, but have been previously elusive in solar models.
- The high-resolution model consists of a 1,024 x 512 x 512 3D mesh that computes the evolution of solar plasma on 1,024 processors running in parallel on the NASA's Pleiades supercomputer and running over hundreds of hours to simulate continuous solar convection.

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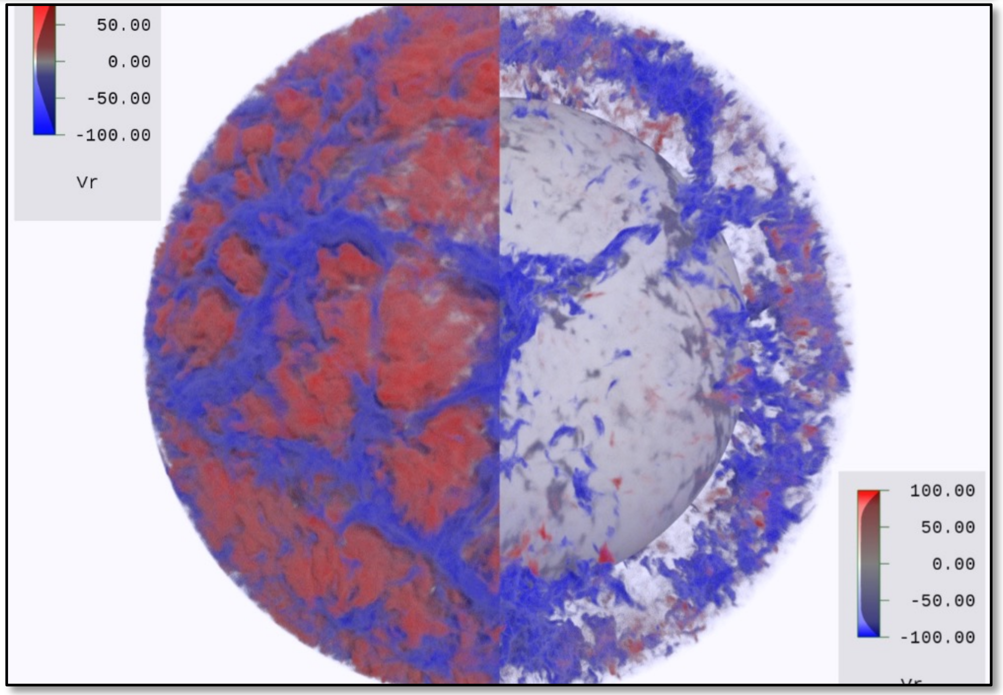
IMPACT: These high-resolution, 3D global models offer a window into the turbulent structures responsible for shaping multiscale convection on the Sun.

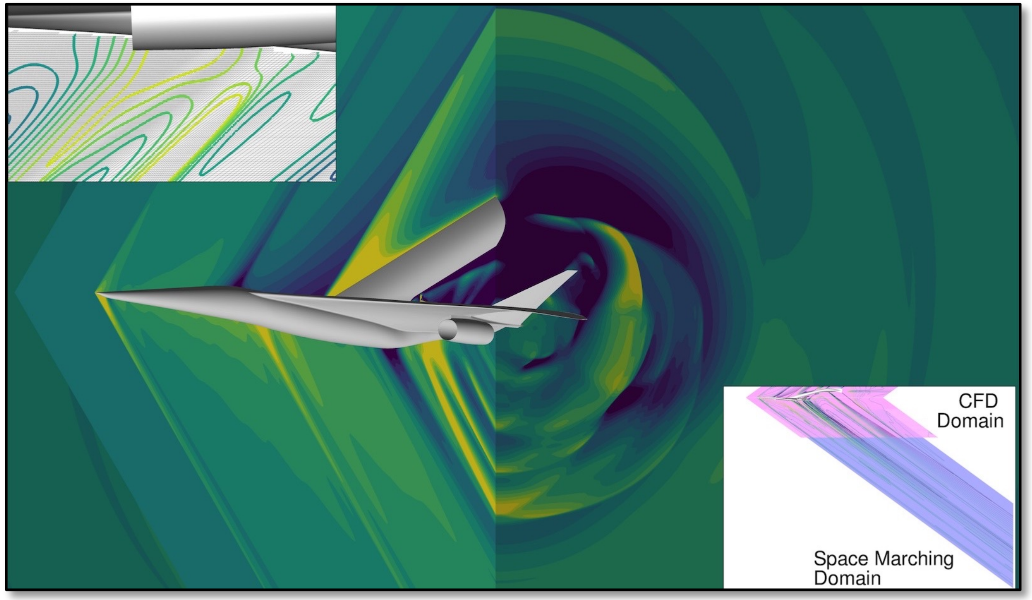


A 3D visualization of radial velocity in the computational domain showing convective cells in detail. The left side of the image shows weaker flows, whereas the right side highlights the strong intergranular downflows. *Andrey Stejko, New Jersey Institute of Technology; Timothy Sandstrom, NASA/Ames*

Preparing the X-59 Quiet Supersonic Aircraft for Flight*

- NASA's X-59 Quiet SuperSonic Technology (QueSST) is an advanced low-boom aircraft concept that will be used to emulate and test the noise generated by future supersonic transport designs. The project goal is to develop an aircraft design that doesn't create an objectionable sonic boom on the ground during supersonic flight.
- The Commercial Supersonic Technologies (CST) project is developing flight planning software that will tell pilots how to fly the aircraft to achieve a target ground-level noise level. Researchers at NASA Ames are using the Agency's Cart3D and Launch Ascent and Vehicle Aerodynamics (LAVA) flow solvers to build a database of thousands of high-fidelity computational fluid dynamics (CFD) simulations that will be used to develop the flight planning tool.
- The LAVA team developed a space marching technique that can be coupled to the CFD to significantly reduce the computational domain, reducing by a factor of two the computational resources required to get a high-fidelity CFD solution. The Cart3D team performed the first fully integrated design optimization of the ground level noise, providing insight into the best ways to manipulate the aircraft's control surfaces for minimum noise impact.
- These improvements will be used to help develop the X-59 advanced flight planning software and to increase the understanding of the relation between changes in the flight parameters and their effect on the ground-level noise.

IMPACT: The design validation and flight prediction database produced for the X-59 project supports NASA's Innovation in Commercial Supersonic Aircraft strategic goals for the Aeronautics Research Mission Directorate.



Visualization of the pressure wave radiating from the low-boom concept aircraft wind tunnel model. Dark blue denotes low pressure, yellow denotes higher pressure. Top left: Solution-adapted Mach-aligned off-body. Bottom right: Relative sizes of the near field computational fluid dynamics domain (pink) and the space marching domain (blue). *Jeffery Housman, NASA/Ames*

** HECC provided supercomputing resources and services in support of this work.*

Papers

- “**Stellar Energetic Particle Transport in the Turbulent and CME-Disrupted Stellar Wind of AU Microscopii**,” F. Fraschetti, et al., The Astrophysical Journal, vol. 937, no. 126, October 1, 2022. *
https://iopscience.iop.org/article/10.3847/1538-4357/ac86d7/pdf
- “**Release of TESS Objects of Interest from TESS-SPOC Sectors 48 to 50 Full Frame Images**,” K. Nguyen, et al., Research Notes of the American Astronomical Society, vol. 6, no. 10, October 2022. *
https://iopscience.iop.org/article/10.3847/2515-5172/ac983a/meta
- “**Host Transcriptional Responses in Nasal Swabs Identify Potential SARS-CoV-2 Infection in PCR Negative Patients**,” A. Saravia-Butler, et al., iScience, vol. 25, issue 11, published online October 7, 2022. *
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- “**Multi-year Observations Reveal a Larger than Expected Autumn Respiration Signal Across Northeast Eurasia**,” B. Byrne, et al., Biogeosciences, vol. 19, issue 19, October 12, 2022. *
https://bg.copernicus.org/articles/19/4779/2022/
- “**Asteroid Interception and Disruption for Terminal Planetary Defense**,” P. Lubin, A. Cohen, Advances in Space Research, available online October 13, 2022. *
https://www.sciencedirect.com/science/article/pii/S0273117722009395
- “**A Sub-Neptune Transiting the Young Field Star HD 18599 at 40 pc**,” J. de Leon, et al., arXiv:2210.08179 [astro-ph.EP], October 15, 2022. *
https://arxiv.org/abs/2210.08179

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- “**Occurrence Rate of Hot Jupiters around Early-Type M Dwarfs Based on TESS Data**,” T. Gan, et al., arXiv:2210.08313 [astro-ph.EP], October 15, 2022. *
https://arxiv.org/abs/2210.08313
- “**Hybrid Simulations of the Cusp and Dayside Magnetosheath Dynamics Under Quasi-Radial Interplanetary Magnetic Fields**,” J. Ng, et al., Journal of Geophysical Research: Space Physics, vol. 127, issue 10, October 17, 2022. *
https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2022JA030359
- “**Stellar Feedback-Regulated Black Hole Growth: Driving Factors from Nuclear to Halo Scales**,” L. Byrne, et al., arXiv:2210.09320 [astro-ph.GA], October 17, 2022. *
https://arxiv.org/abs/2210.09320
- “**TOI-969: A Late-K Dwarf with a Hot Mini-Neptune in the Desert and an Eccentric Cold Jupiter**,” J. Lillo-Box, et al., arXiv:2210.08996 [astro-ph.EP], October 17, 2022. *
https://arxiv.org/abs/2210.08996
- “**Characterization of the HD 108236 System with CHEOPS and TESS. Confirmation of a Fifth Transiting Planet**,” S. Hoyer, et al., arXiv:2210.08912 [astro-ph.EP], October 17, 2022. *
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- “**TOI-1136 is a Young, Coplanar, Aligned Planetary System in a Pristine Resonant Chain**,” F. Dai, et al., arXiv:2210.09283 [astro-ph.EP], October 17, 2022. *
https://arxiv.org/abs/2210.09283

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Papers (cont.)

- “**TOI-3884 b: A Rare 6-R⊕ Planet that Transits a Low-Mass Star with a Giant and Likely Polar Spot**,” J. Almenara, et al., arXiv:2210.10909 [astro-ph.EP], October 19, 2022. *
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- “**A Low-Mass, Pre-Main Sequence Eclipsing Binary in the 40 Myr Columbia Association – Fundamental Stellar Parameters and Modeling the Effect of Star Spots**,” B. Tofflemire, et al., arXiv:2210.10789 [astro-ph.SR], October 19, 2022. *
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- “**A Dynamic Nonlinear Subgrid-Scale Model for Large-Eddy Simulation of Complex Turbulent Flows**,” A. Uzun, M. Malik, NASA/TM-20220013891, October 2022. *
  https://www.researchgate.net/publication/364331005_A_Dynamic_Nonlinear_Subgrid-Scale_Model_for_Large-Eddy_Simulation_of_Complex_Turbulent_Flows
- “**Precise Mass Determination for the Keystone Sub-Neptune Planet Transiting the Mid-Type M Dwarf G 9-40**,” R. Luque, et al., Astronomy & Astrophysics, vol. 666, October 21, 2022.
  https://www.aanda.org/articles/aa/full_html/2022/10/aa44426-22/aa44426-22.html
- “**Faster Tropical Upper Stratospheric Upwelling Drives Changes in Ozone Chemistry**,” S. Strahan, et al., Geophysical Research Letters, vol. 49, issue 20, October 25, 2022. *
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Papers (cont.)

- "**Comprehensive Study of HCN: Potential Energy Surfaces, State-to-State Kinetics, and Master Equation Analysis**," M. Priyadarshini, et al., The Journal of Physical Chemistry A, published online October 26m 2022. *
https://pubs.acs.org/doi/abs/10.1021/acs.jpca.2c03959
- "**Structure and Computational Electrophysiology of Ac-LS3, a Synthetic Ion Channel**," M. Wilson, A. Pohorille, The Journal of Physical Chemistry B, published online October 28, 2022. *
https://pubs.acs.org/doi/abs/10.1021/acs.jpcb.2c05965
- "**The HD 93963 A Transiting System: A 1.04 d Super-Earth and a 3.65 d Sub-Neptune Discovered by TESS and CHEOPS**," L. Serrano, et al., Astronomy & Astrophysics, vol. 667, October 28, 2022. *
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News and Events

- **Supercomputer Simulations Reveal How the Sun Accelerates Charged Particles**, *physicsworld*, October 6, 2022—Researchers from Columbia University have used supercomputers to gain insights into the origins of the solar wind. The large-scale simulations for this work were performed on NASA's Pleiades supercomputer and the Cori supercomputer at NERSC, using particle-in-cell code across 50,000 to 100,000 CPUs and about 1,500 nodes. https://physicsworld.com/a/supercomputer-simulations-reveal-how-the-sun-accelerates-charged-particles/
- **Ocean-Atmosphere Mashup: A Recipe for Climate Predictions**, *NAS Feature*, October 4, 2022—What happens when scientists cook up a new recipe for understanding the workings of our planet? That's what two teams studying Earth's oceans and atmosphere decided to find out—with help from visualization experts in the NASA Advanced Supercomputing (NAS) Division and the agency's high-performance computing (HPC) resources. https://www.nas.nasa.gov/pubs/stories/2022/feature_ocean_atmosphere_mashup.html

Presentations

- “**Supersonic Parachute Inflation Modeling in LAVA**,” F. Cadieux, NASA Entry Systems Modeling Workshop, October 3-6, 2022.*
- “**Development of HelioPortal to Enable Reliable Forecasts of Solar Activity through Data Assimilation and Machine Learning Approaches**,” I. Kitiashvili, Second International Workshop on Small Satellites for Space Weather Research & Forecasting, Laural, MD, October 3-7, 2022.*
- ”**Progress in Reprocessing the Hyperion/EO-1 Data Set with a Prototype Pipeline for SBG**,” J. Jenkins, 9th Surface Biology and Geology Community Workshop, Washington, D.C., October 12-14, 2022.*
- “**Science Processing Operations Center (SPOC) Status**,” J. Jenkins, TESS Science Team Meeting #29, Virtual, October 13-14, 2022.*
- “**Cart3D-Mphys Integration**,” J. Chiew, MphysWorkshop, Cleveland, OH, October 26, 2022.*

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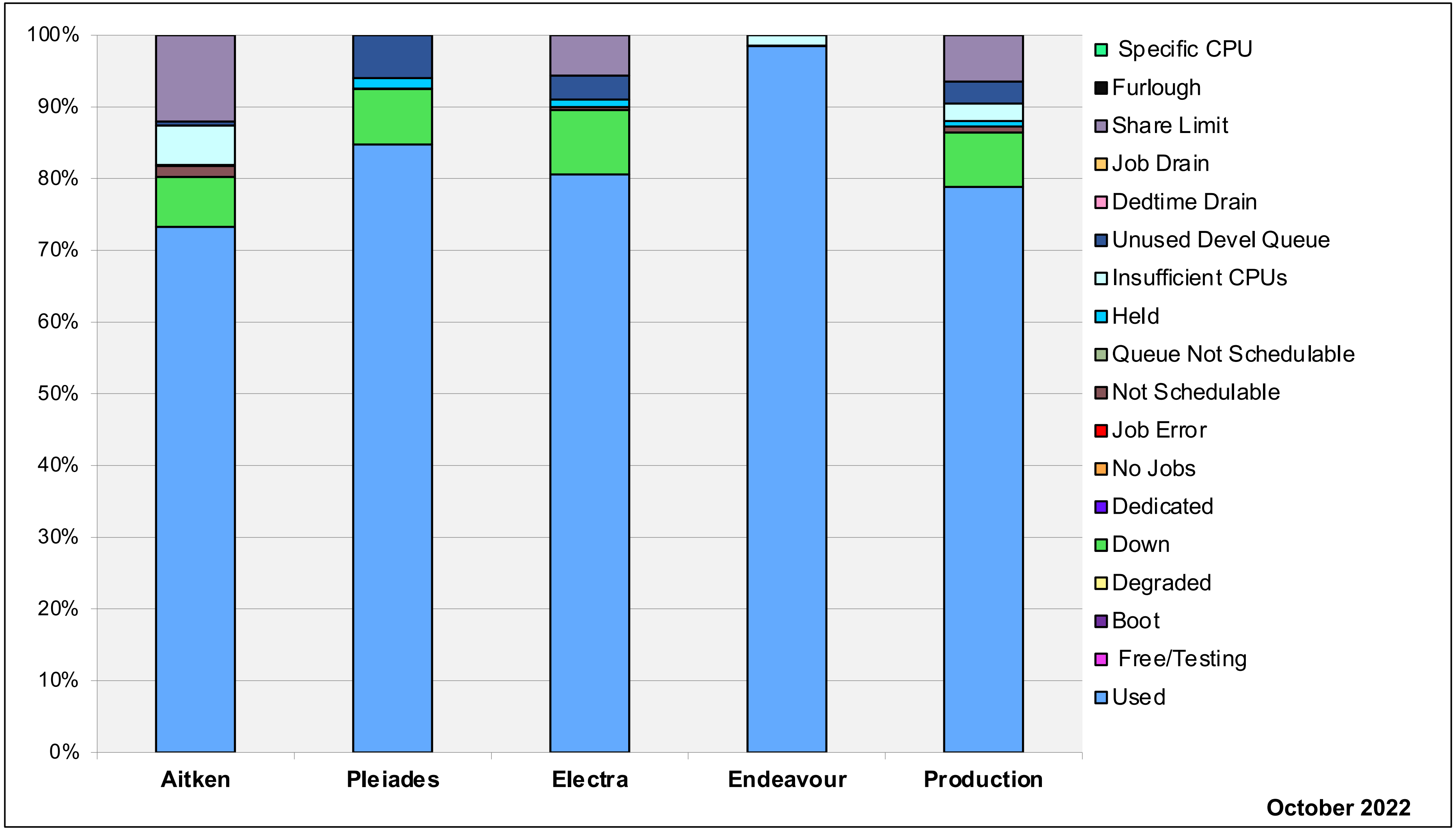
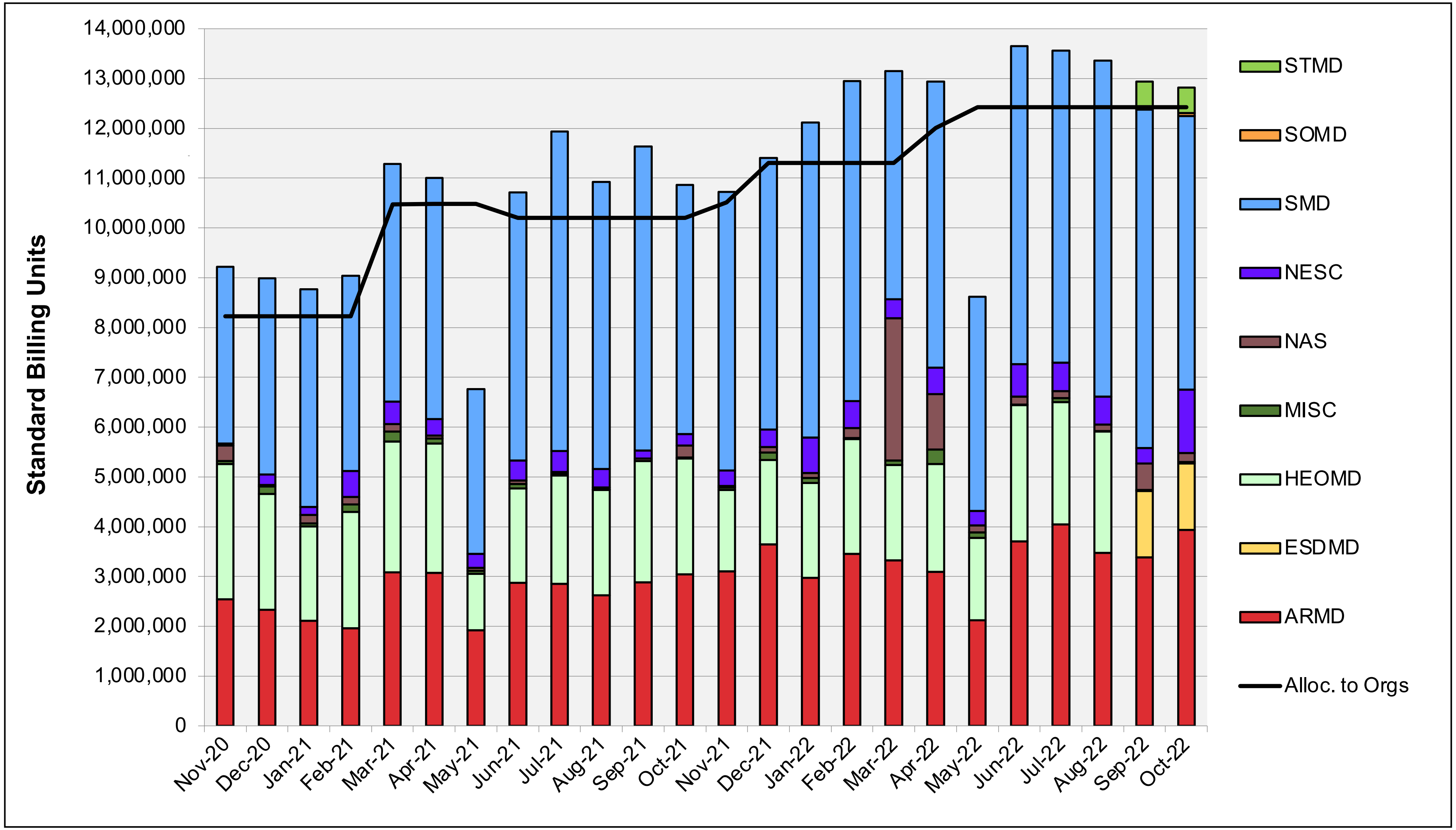
News and Events: Social Media

- **Coverage of NAS Stories**
  - Global Ocean-Atmosphere Simulations (ECCO/GEOS):
    - NAS: Twitter 5 retweets, 2 quote tweets, 7 likes.
    - NASA Supercomputing: Facebook 772 users reached, 43 reactions.

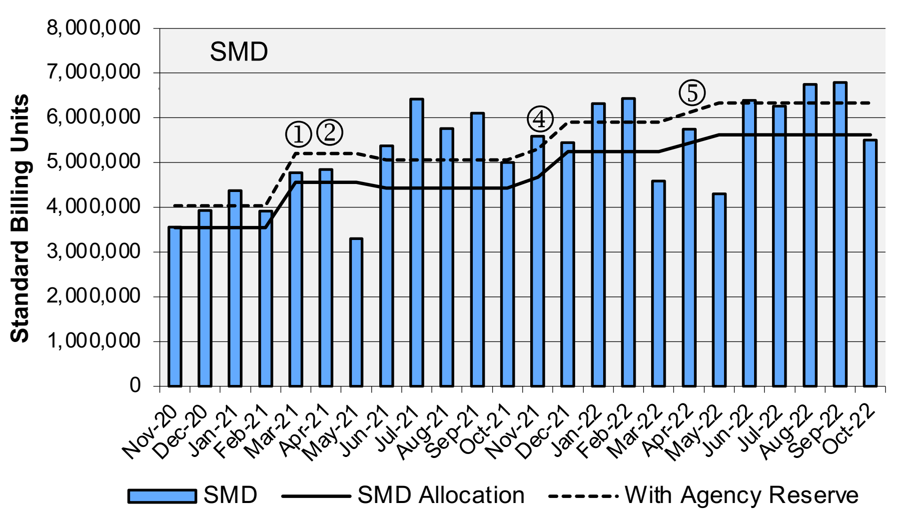
HECC Utilization

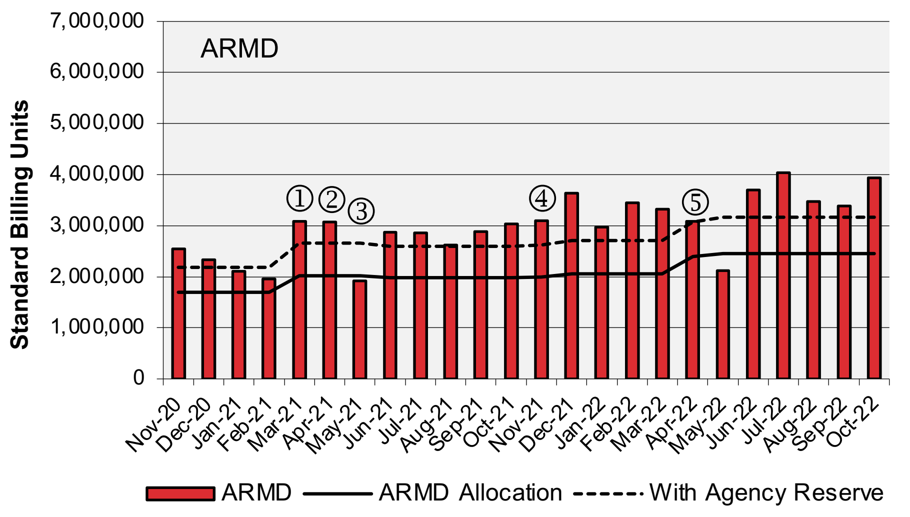


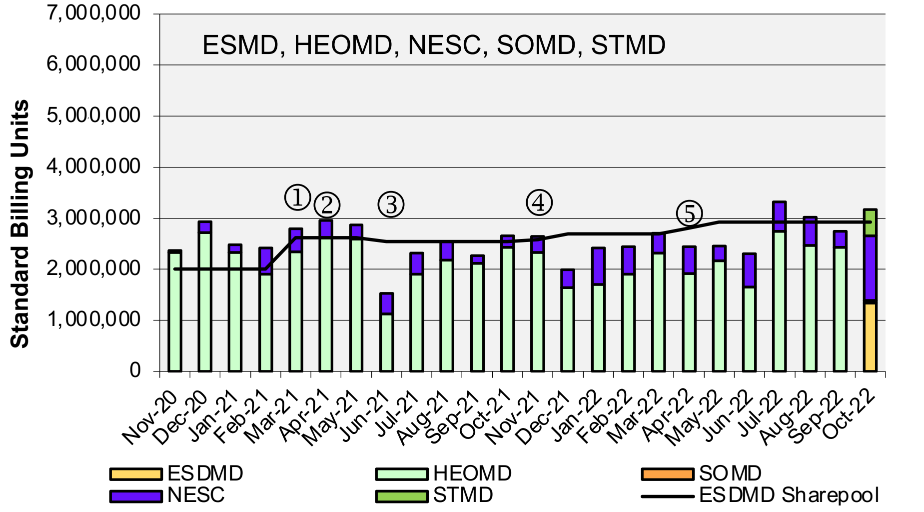
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







① 8 Rome Apollo racks introduced into Aitken

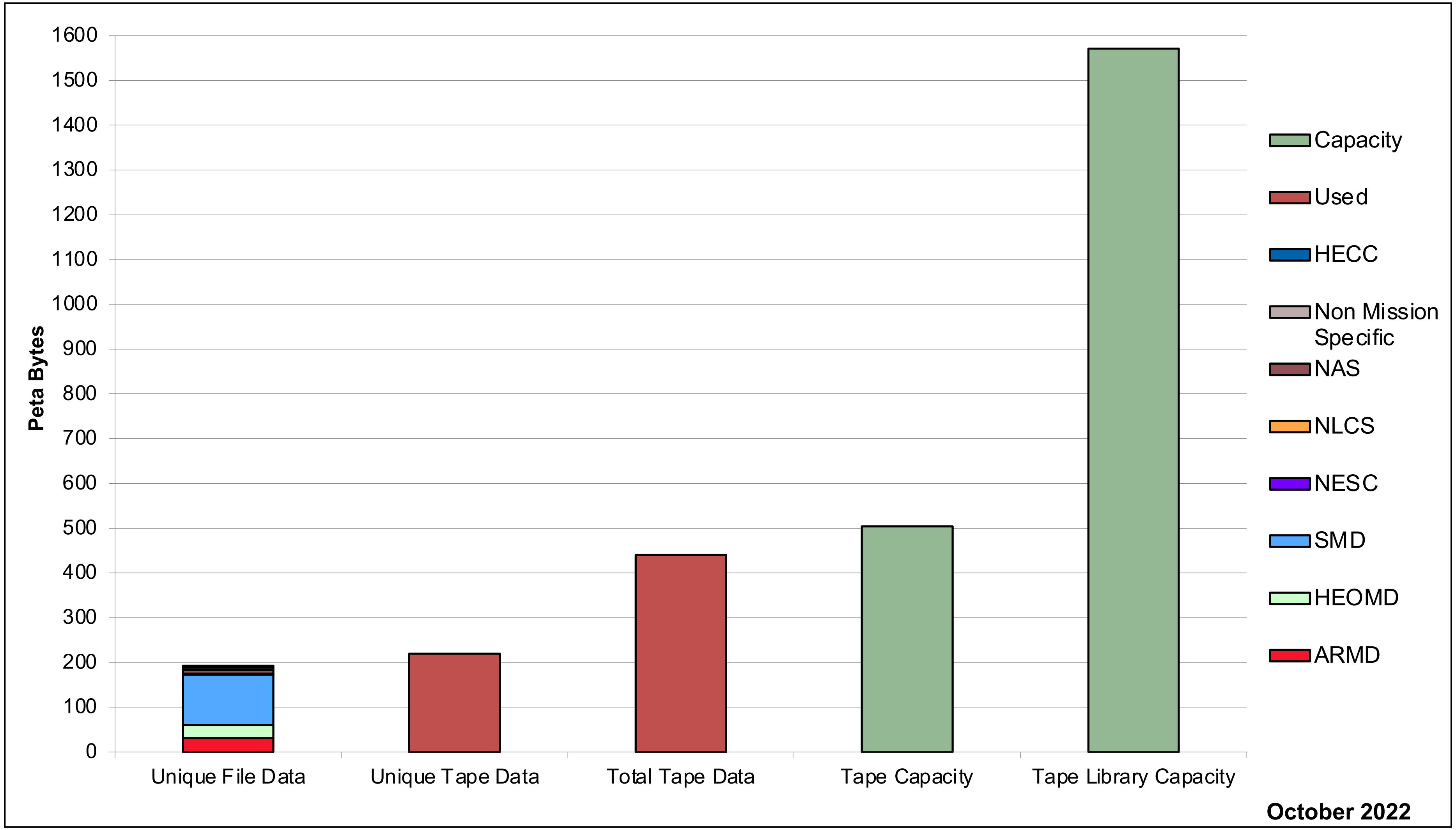
② Endeavour replaced with new hardware

③ Merope retired

④ 4 Rome Apollo Racks added to Aitken

⑤ 4 Rome Apollo Racks added to Aitken

Tape Archive Status



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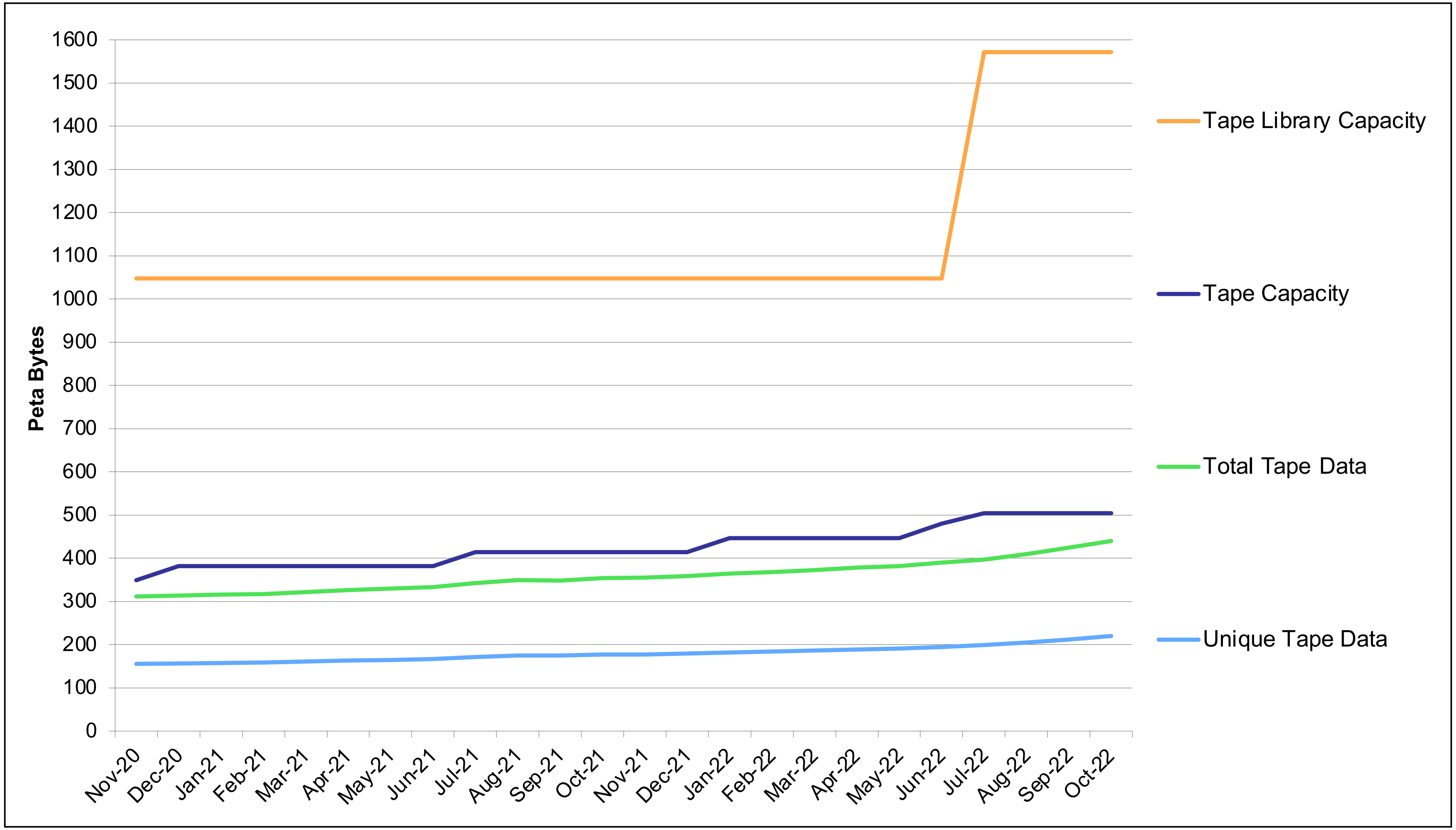
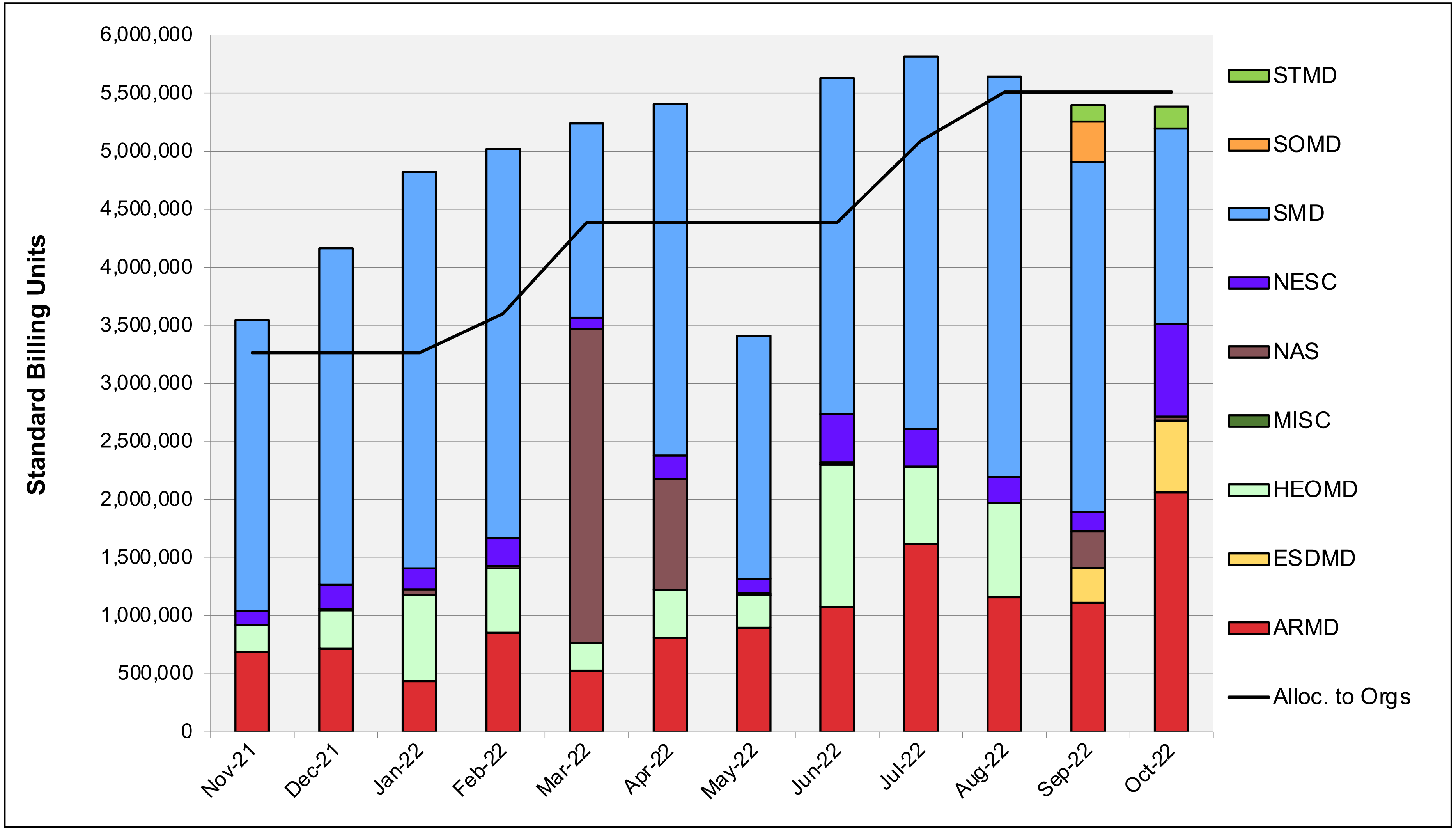
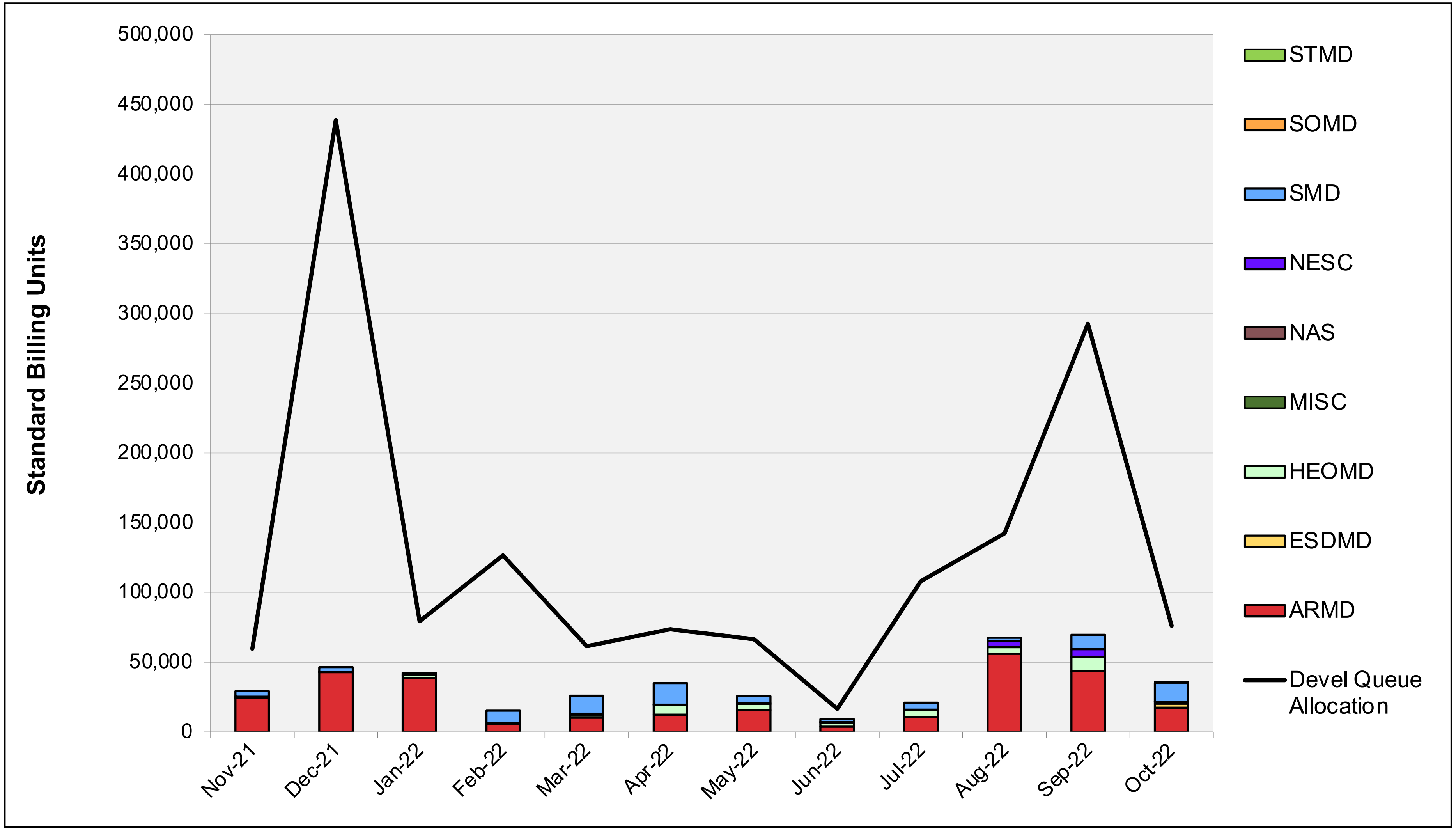


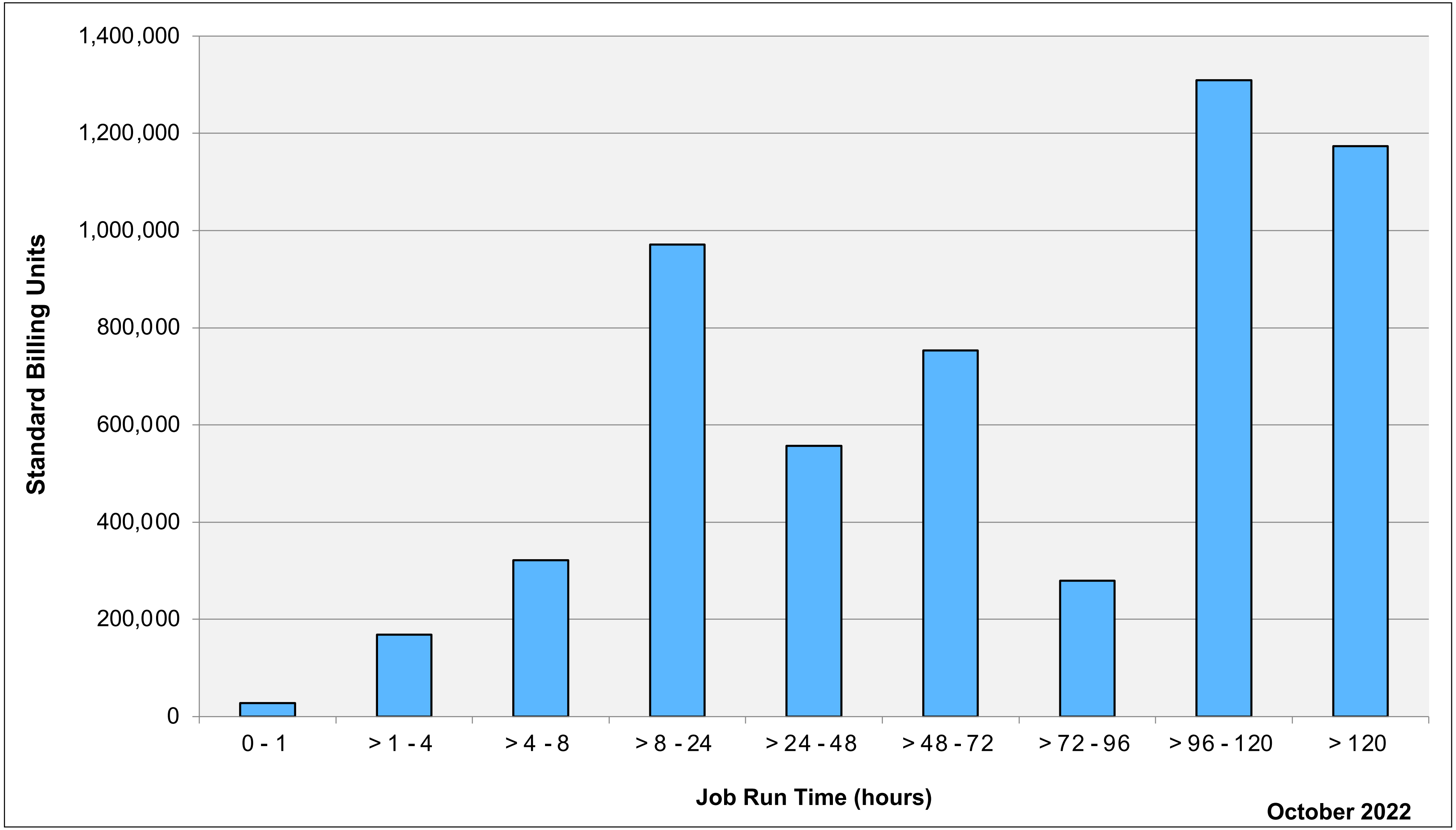
Aitken: SBUs Reported, Normalized to 30-Day Month



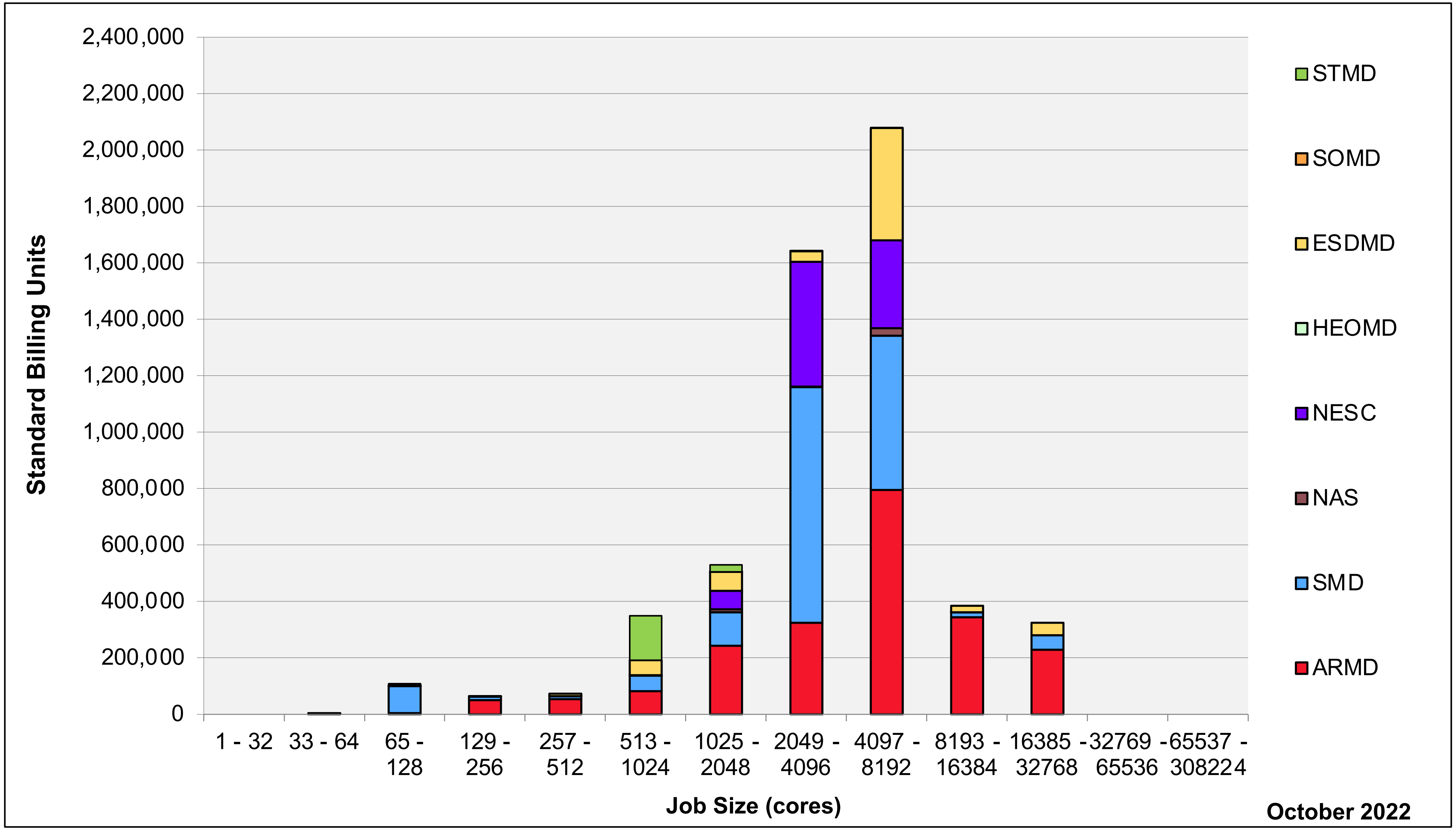
Aitken: Devel Queue Utilization



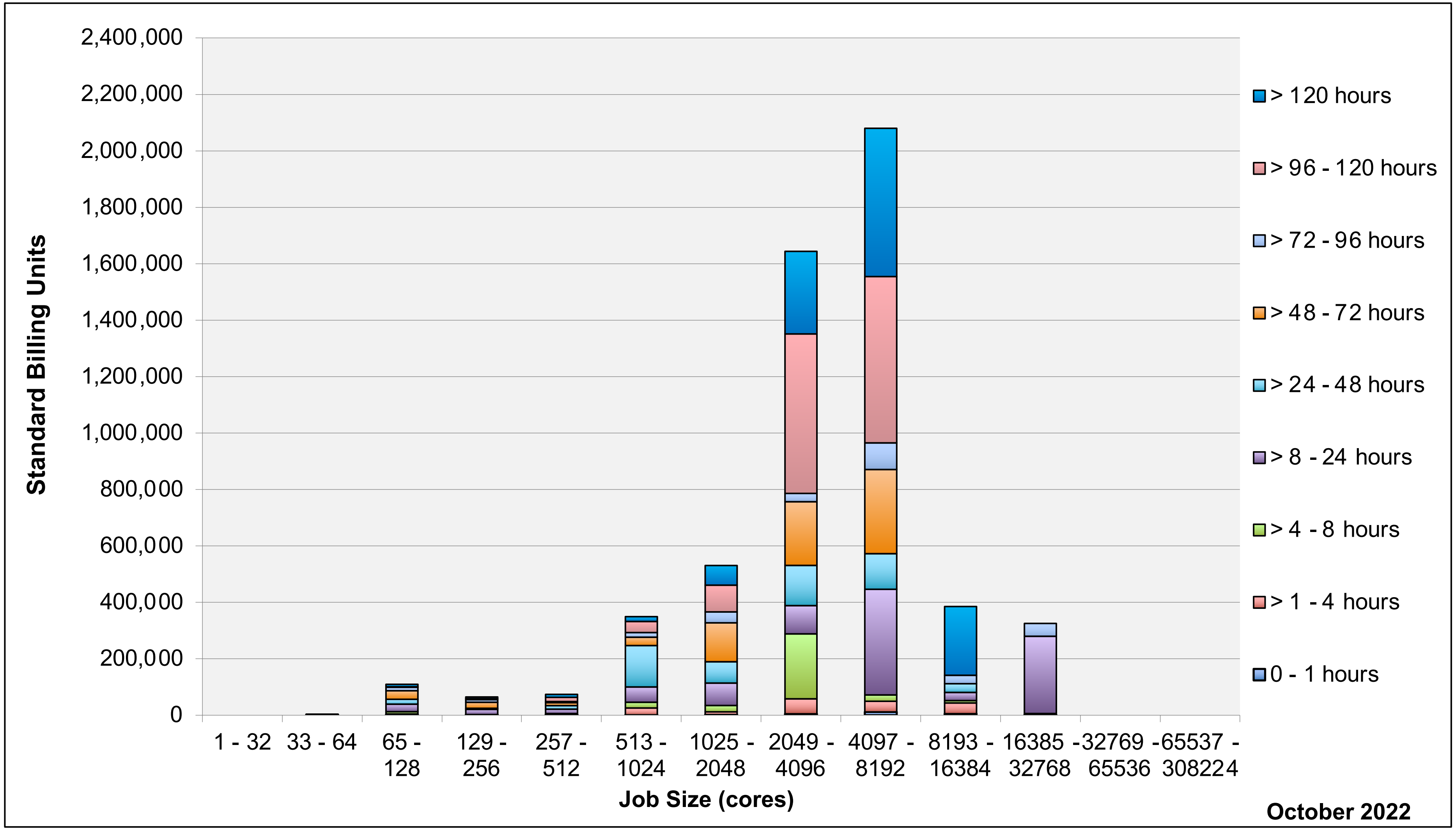
Aitken: Monthly Utilization by Job Length



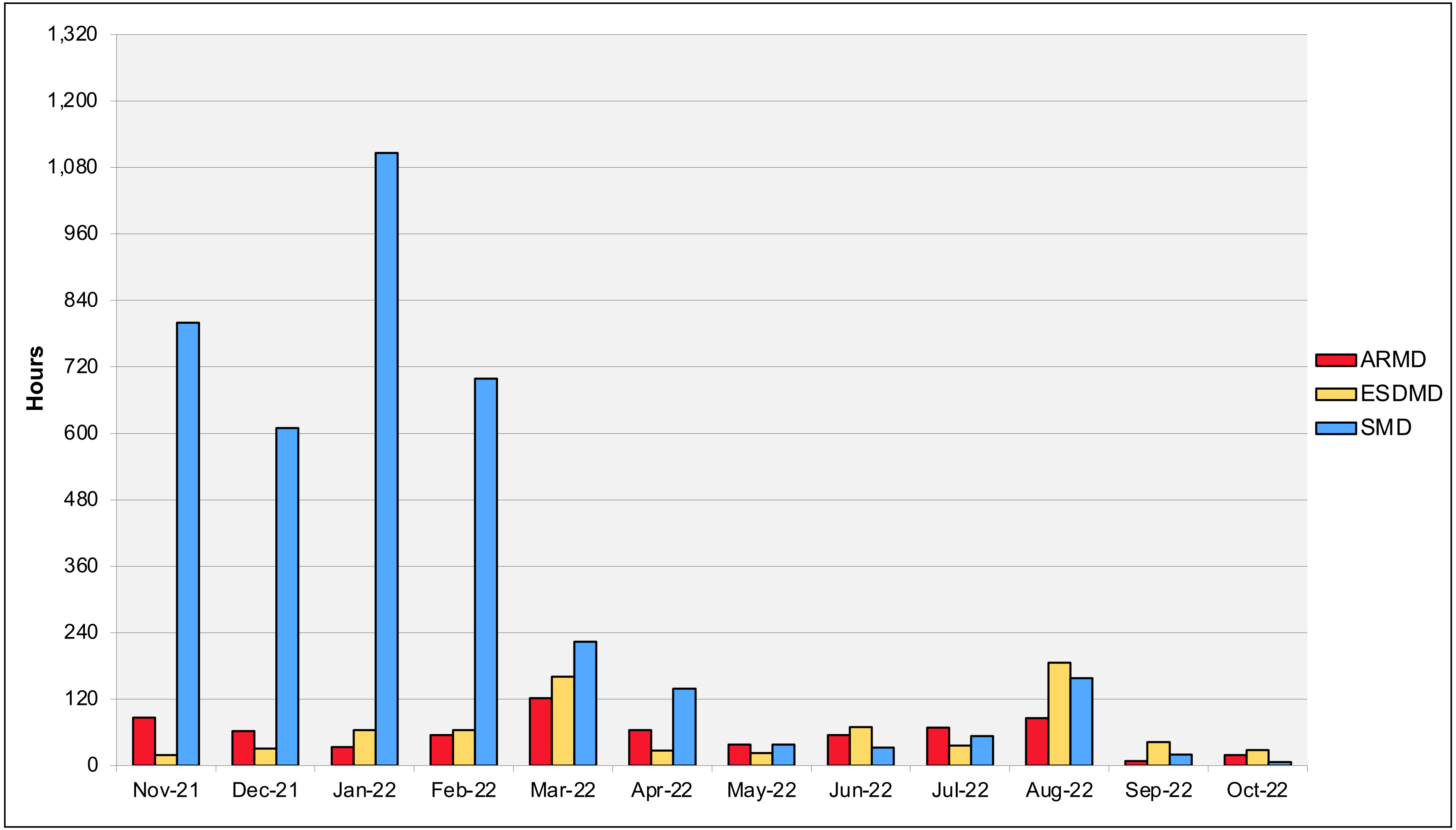
Aitken: Monthly Utilization by Job Size



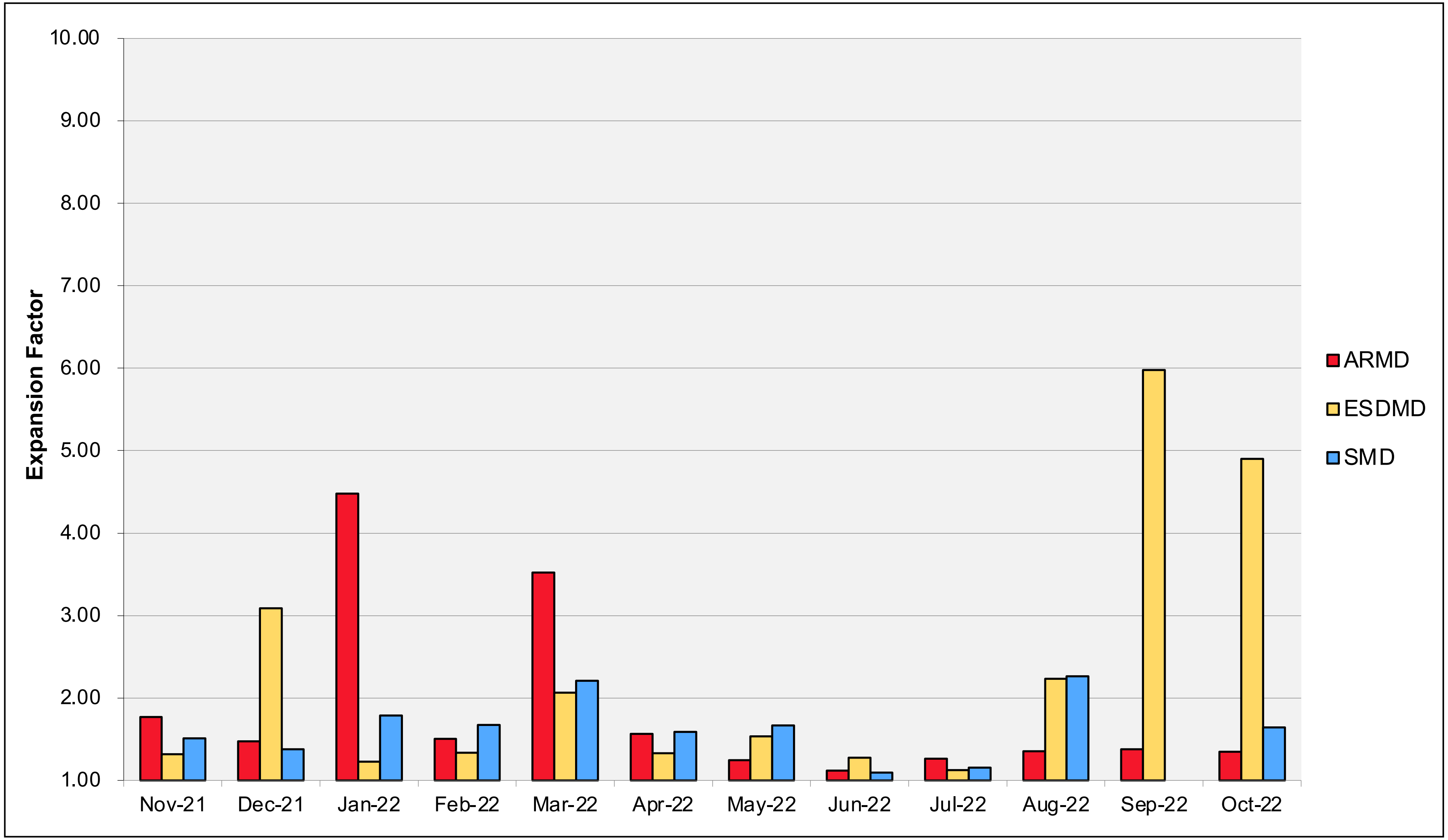
Aitken: Monthly Utilization by Size and Length



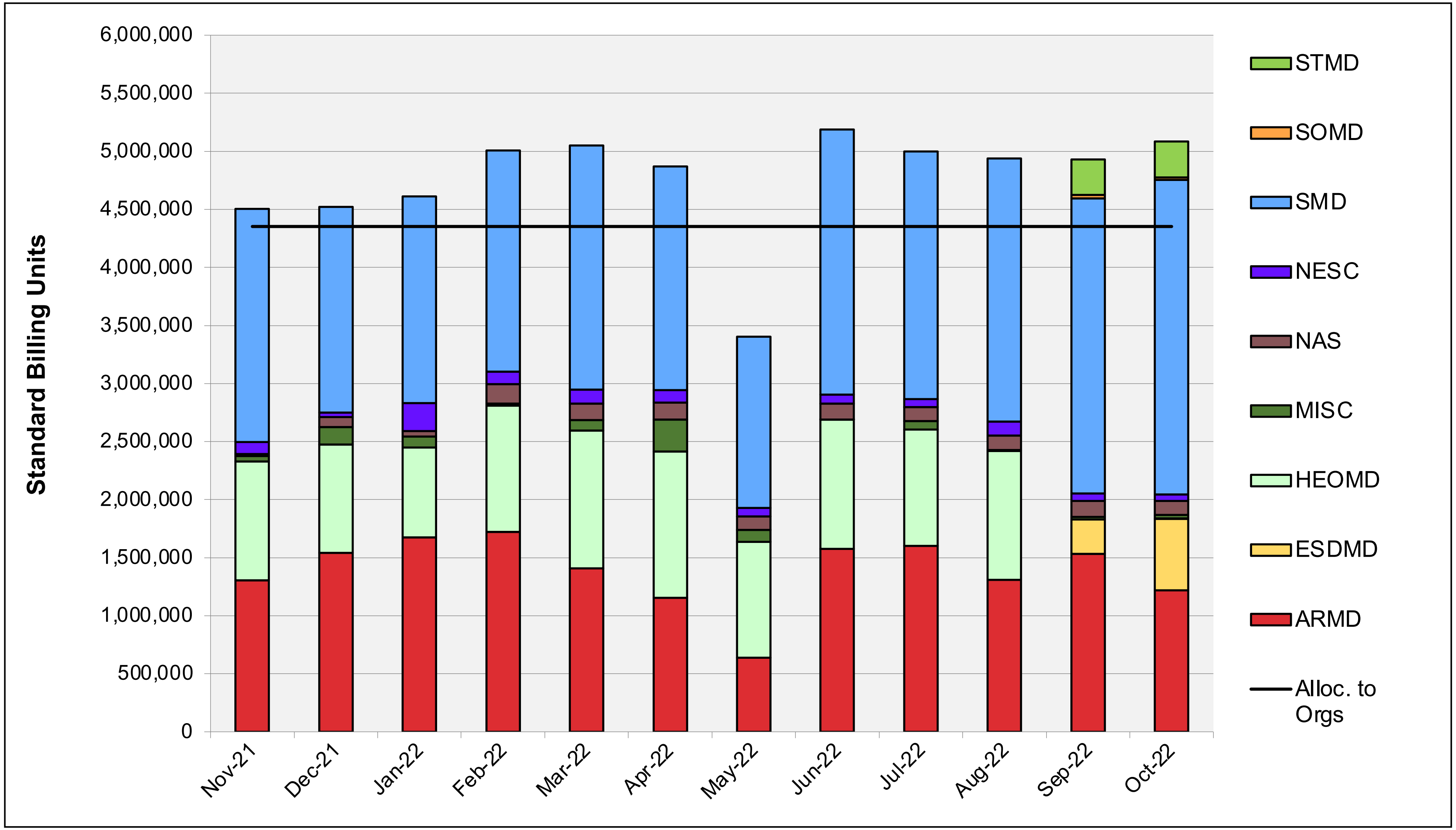
Aitken: Average Time to Clear All Jobs



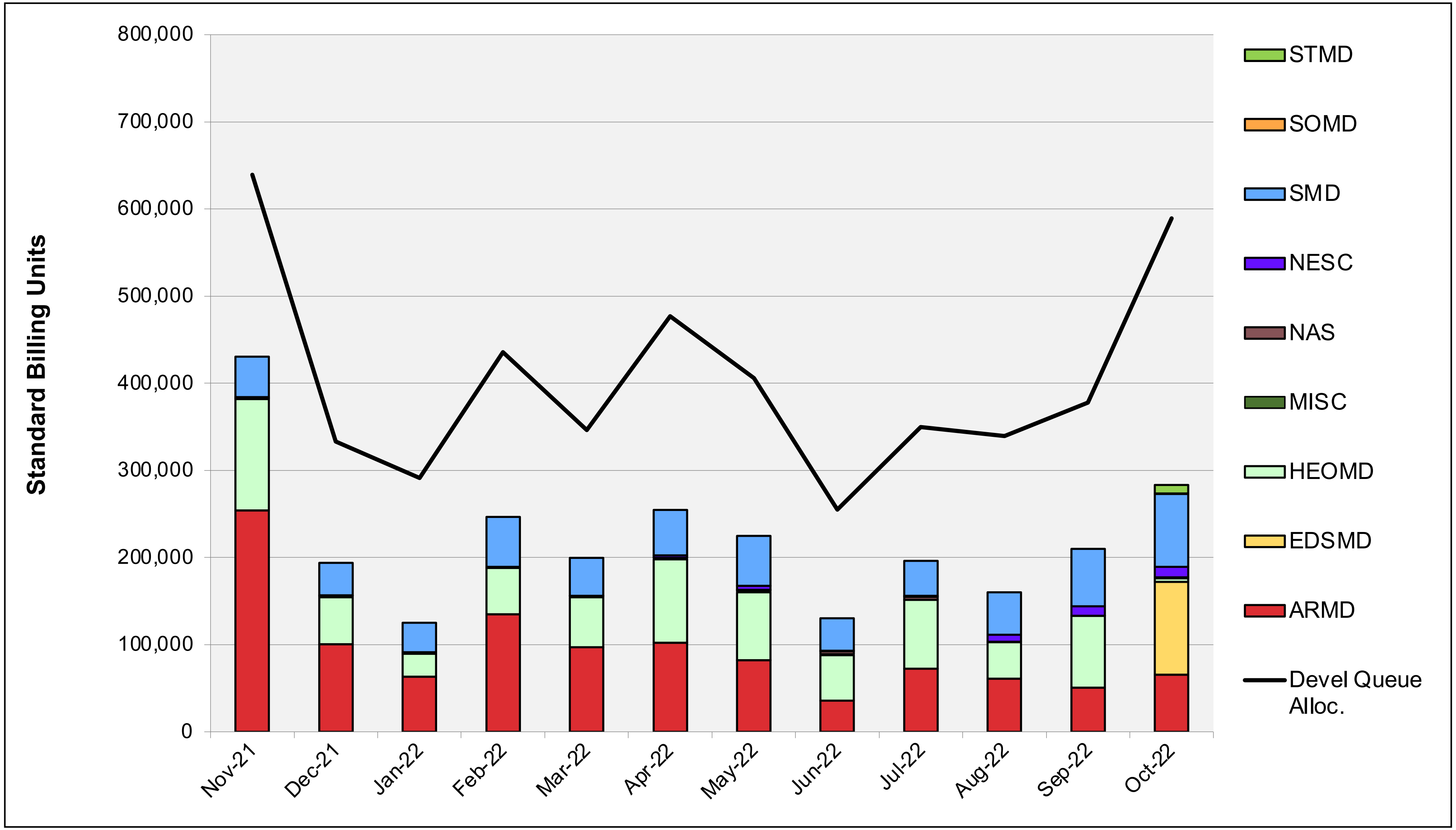
Aitken: Average Expansion Factor



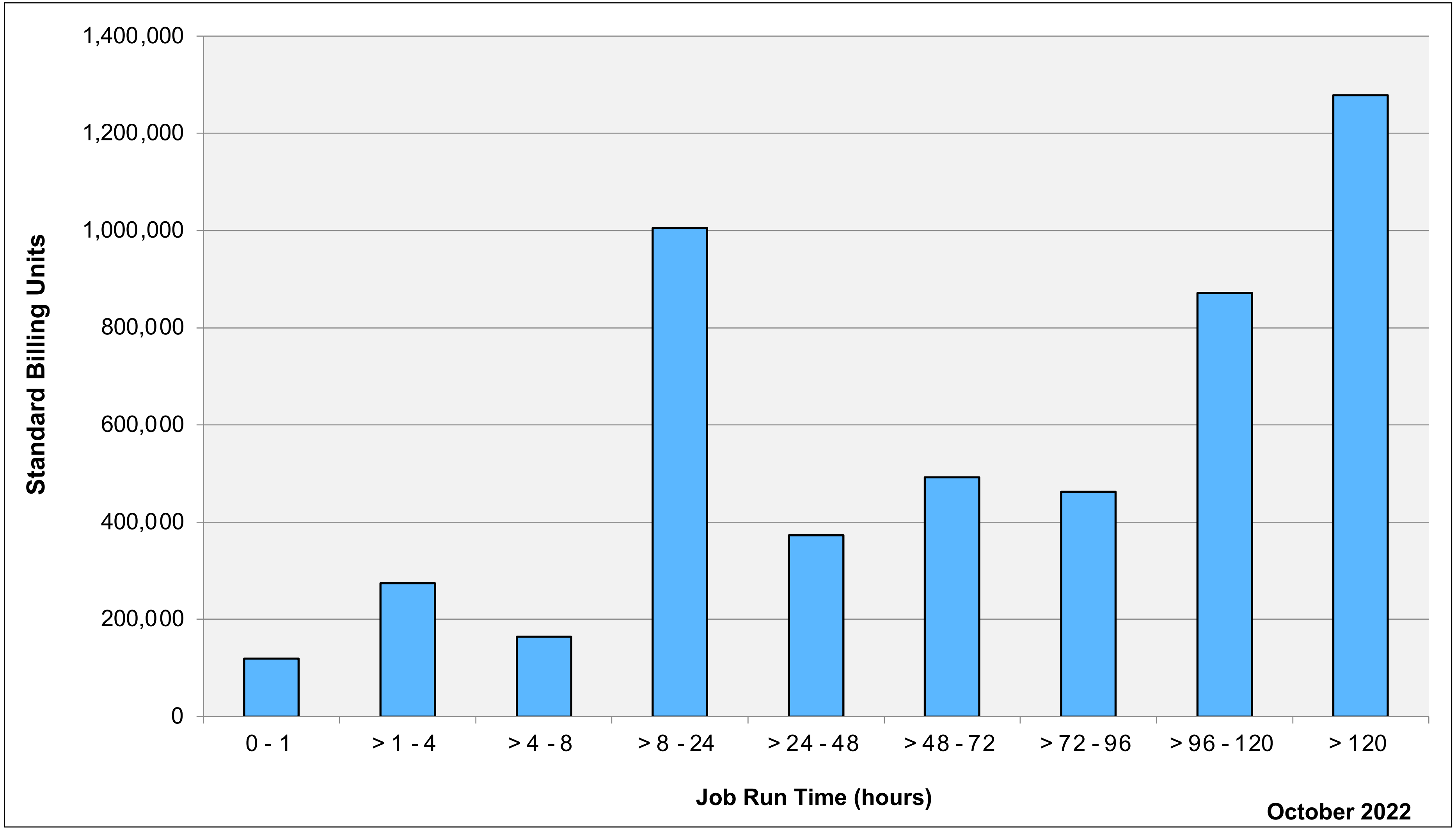
Pleiades: SBUs Reported, Normalized to 30-Day Month



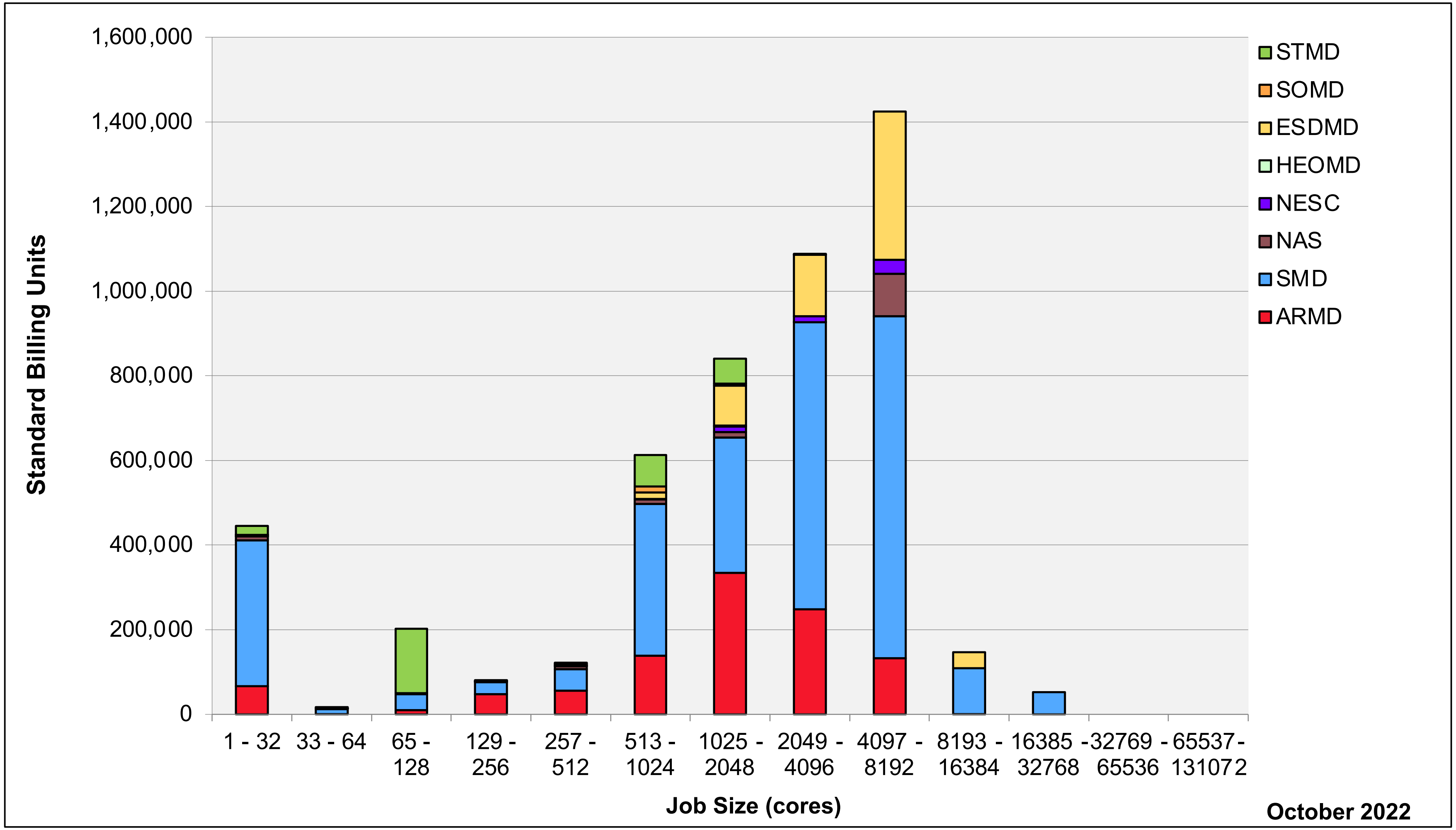
Pleiades: Devel Queue Utilization



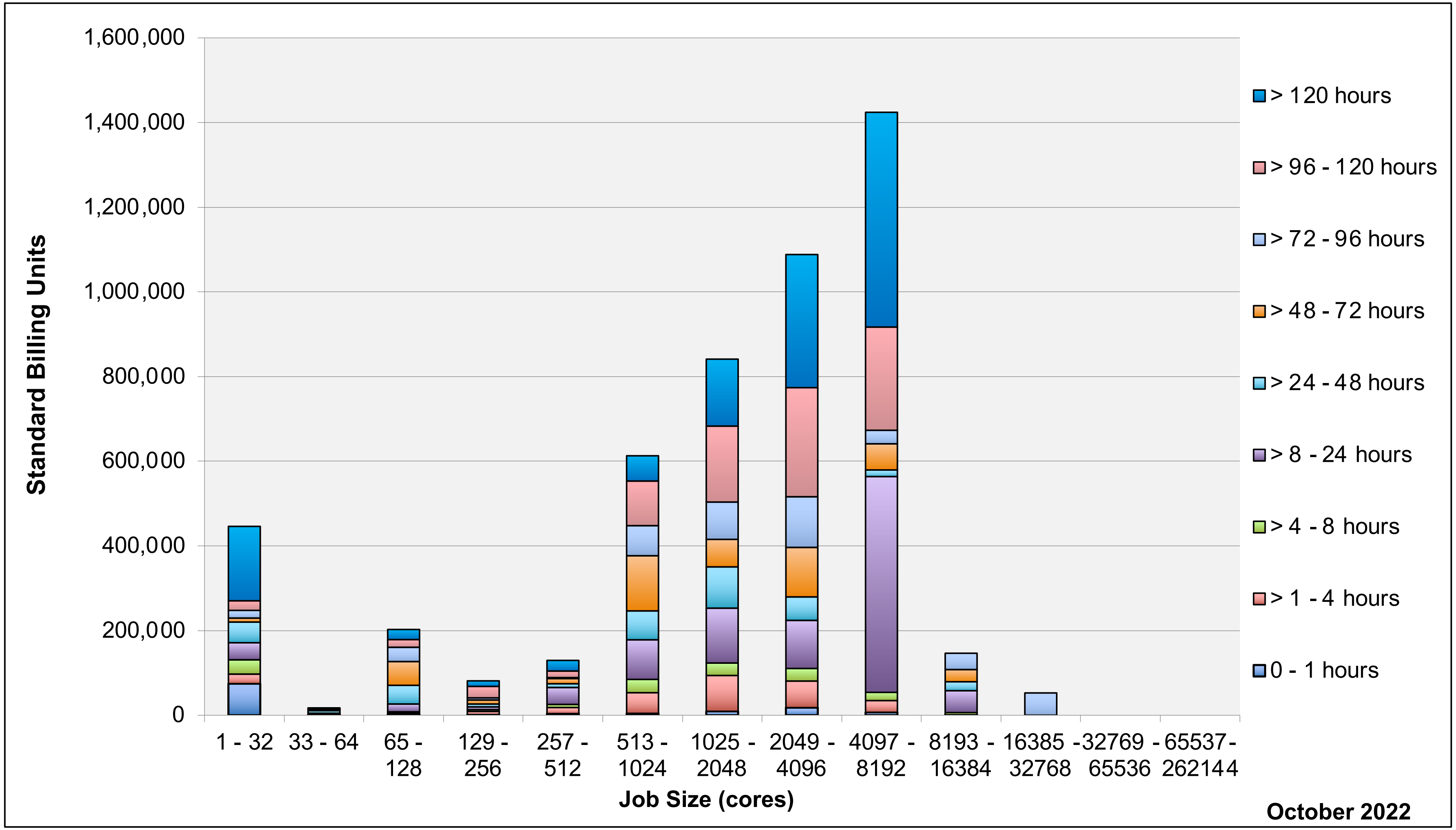
Pleiades: Monthly Utilization by Job Length



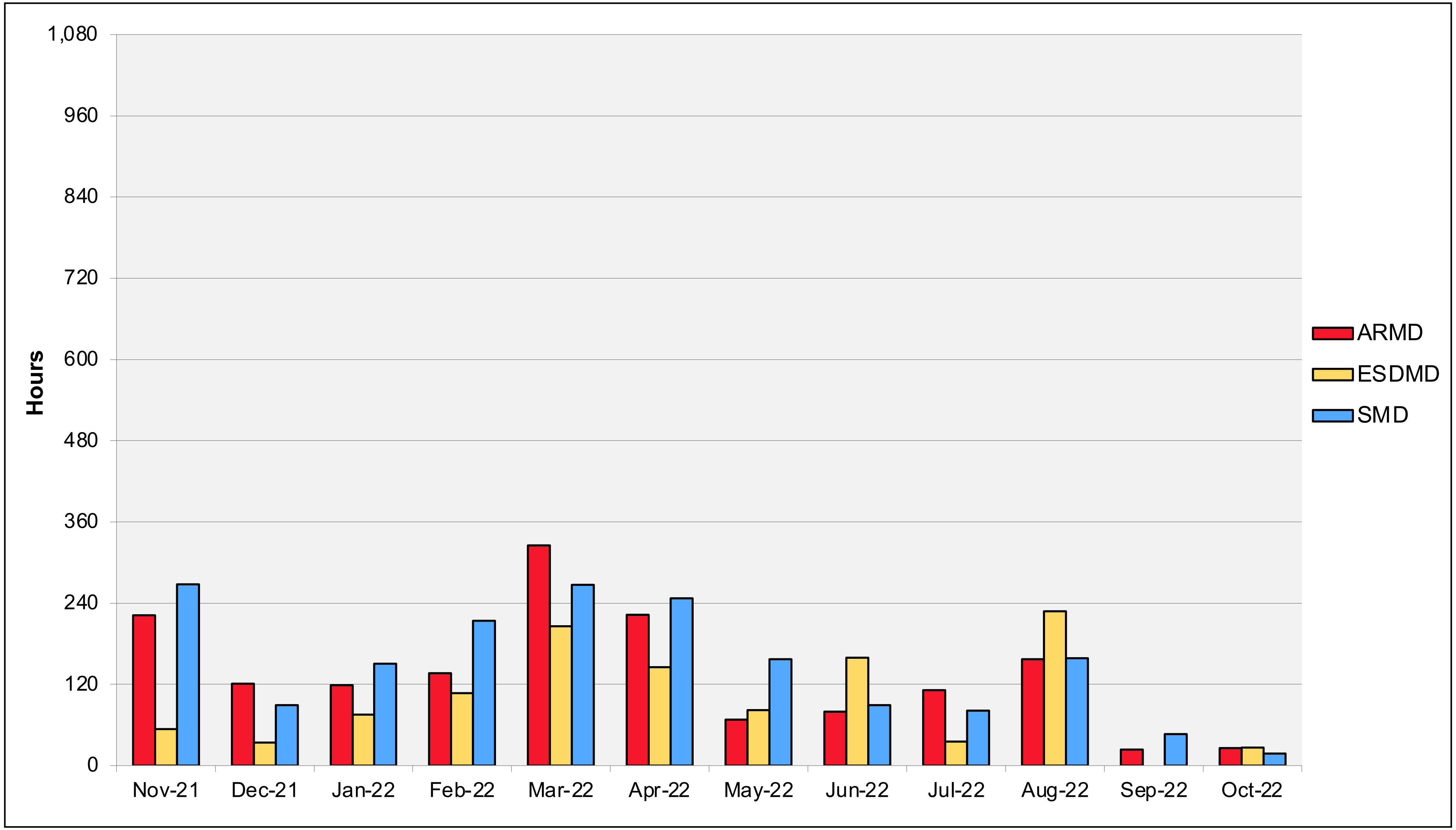
Pleiades: Monthly Utilization by Job Size



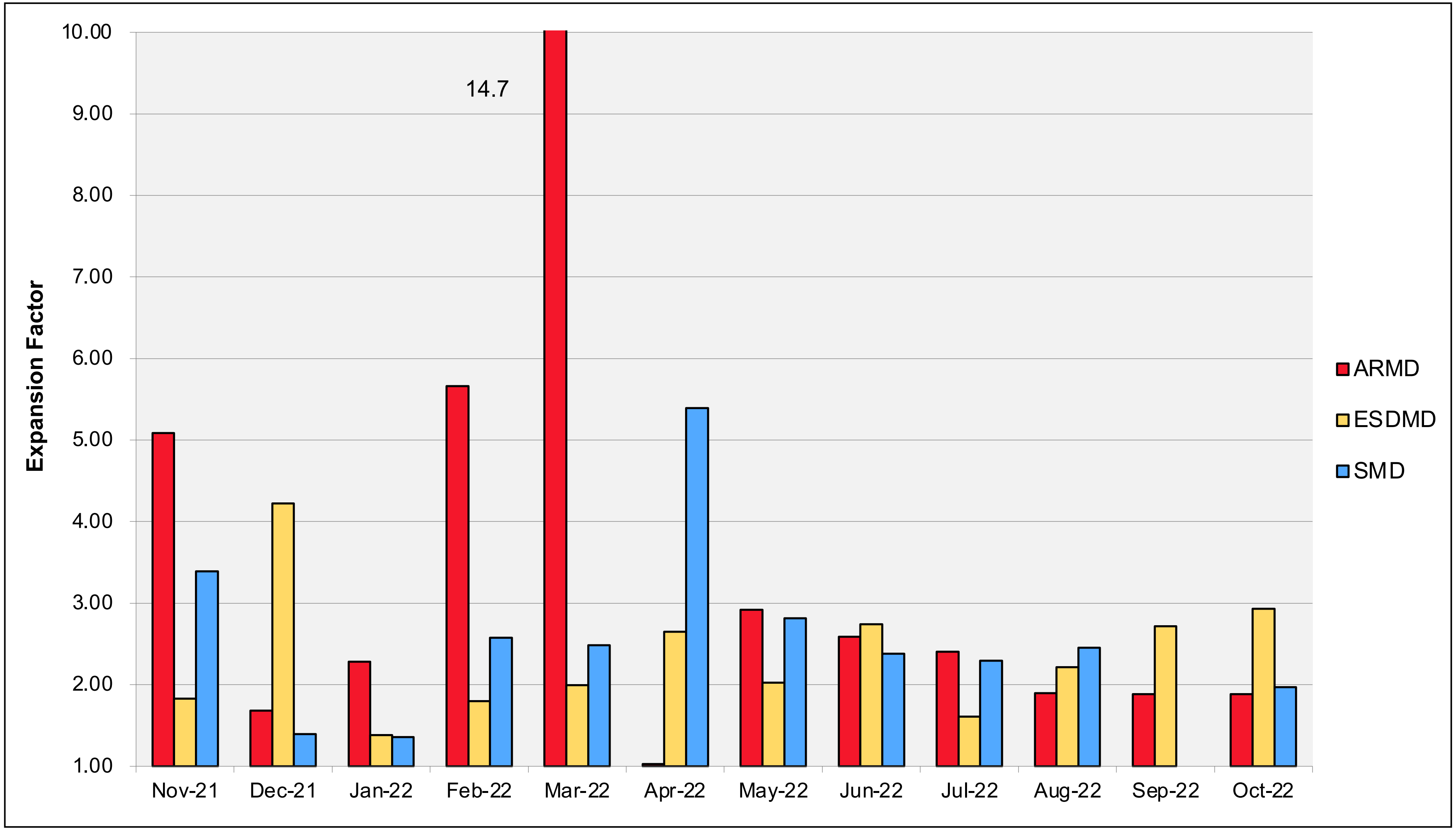
Pleiades: Monthly Utilization by Size and Length



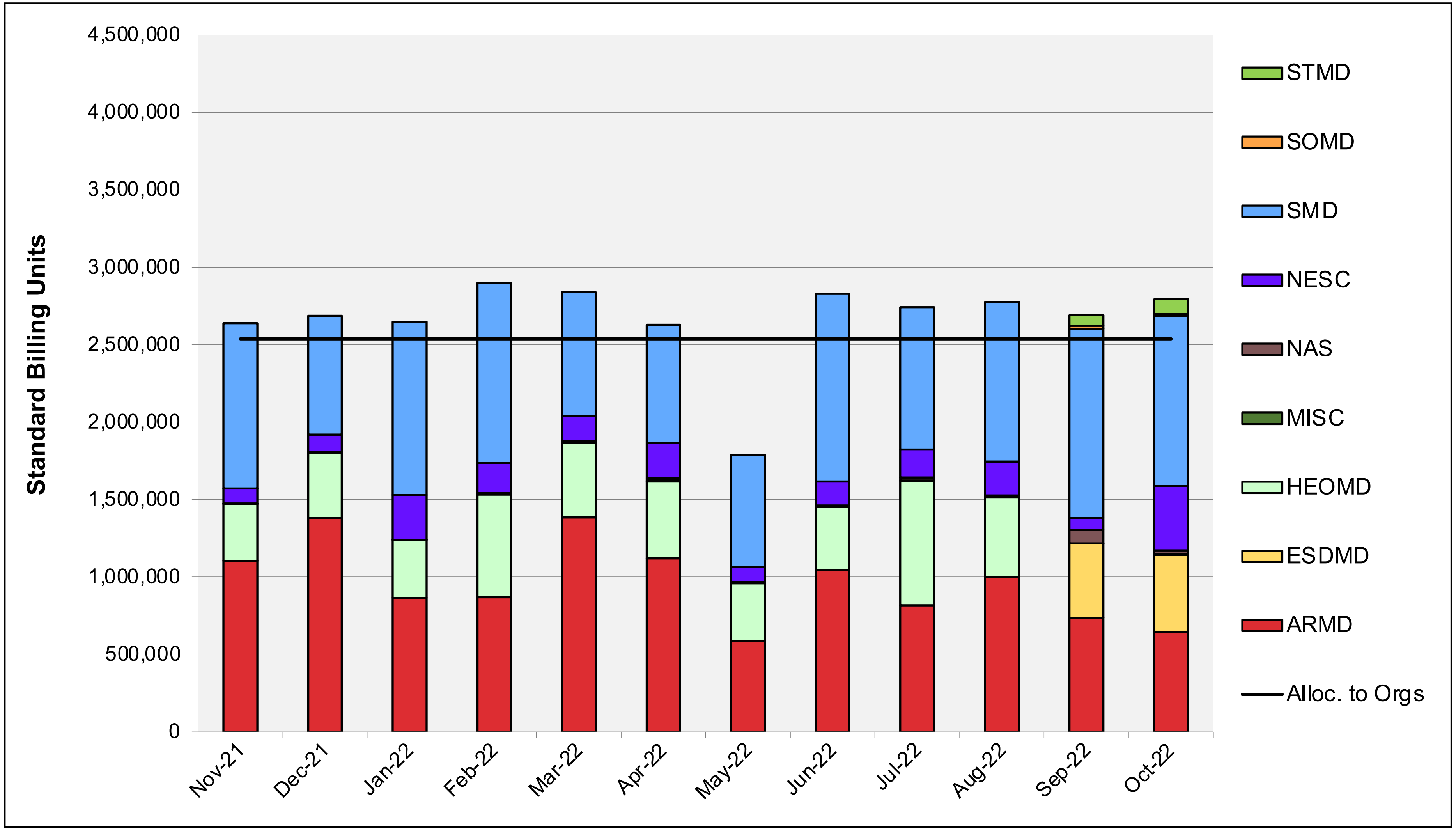
Pleiades: Average Time to Clear All Jobs



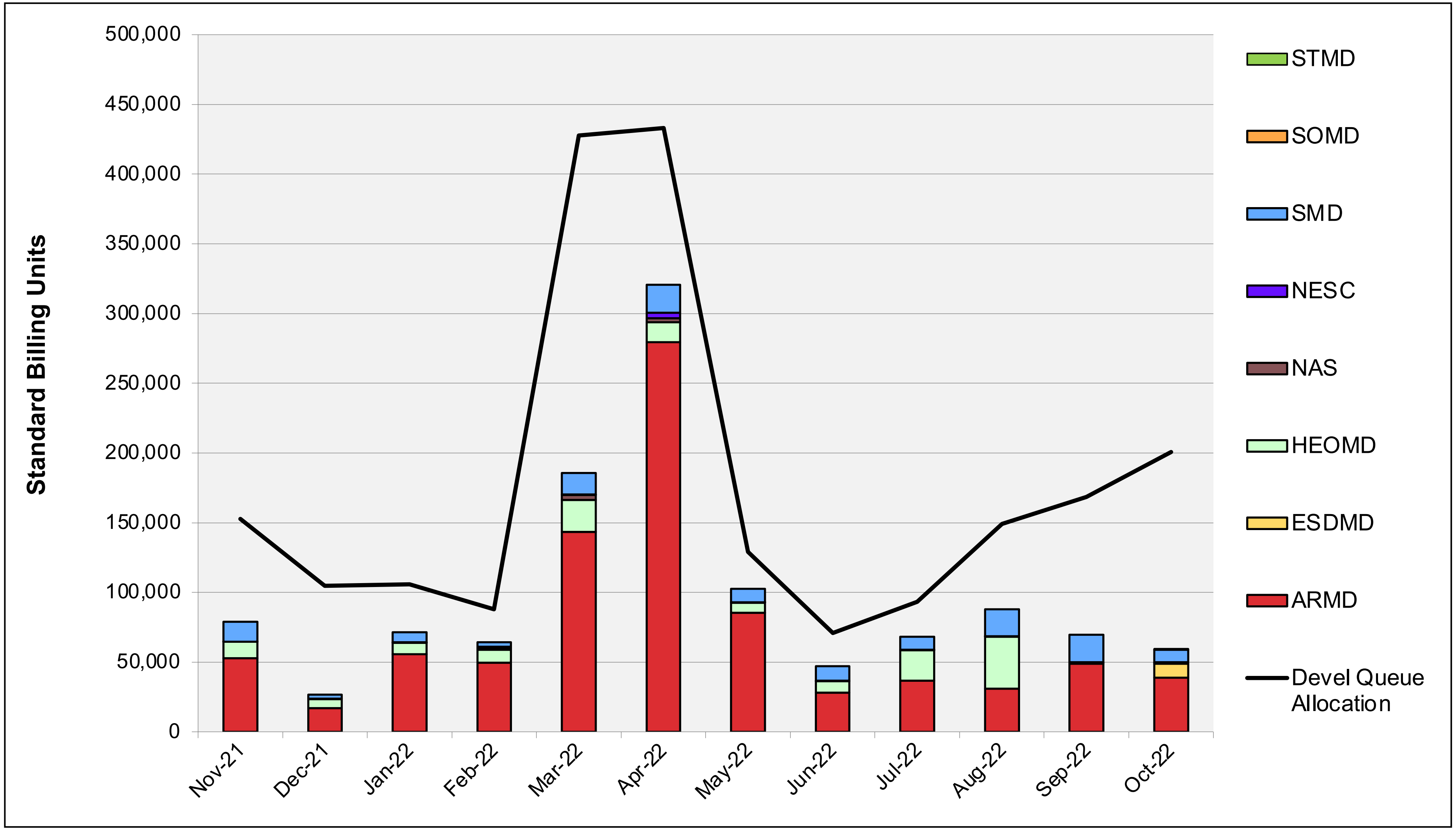
Pleiades: Average Expansion Factor



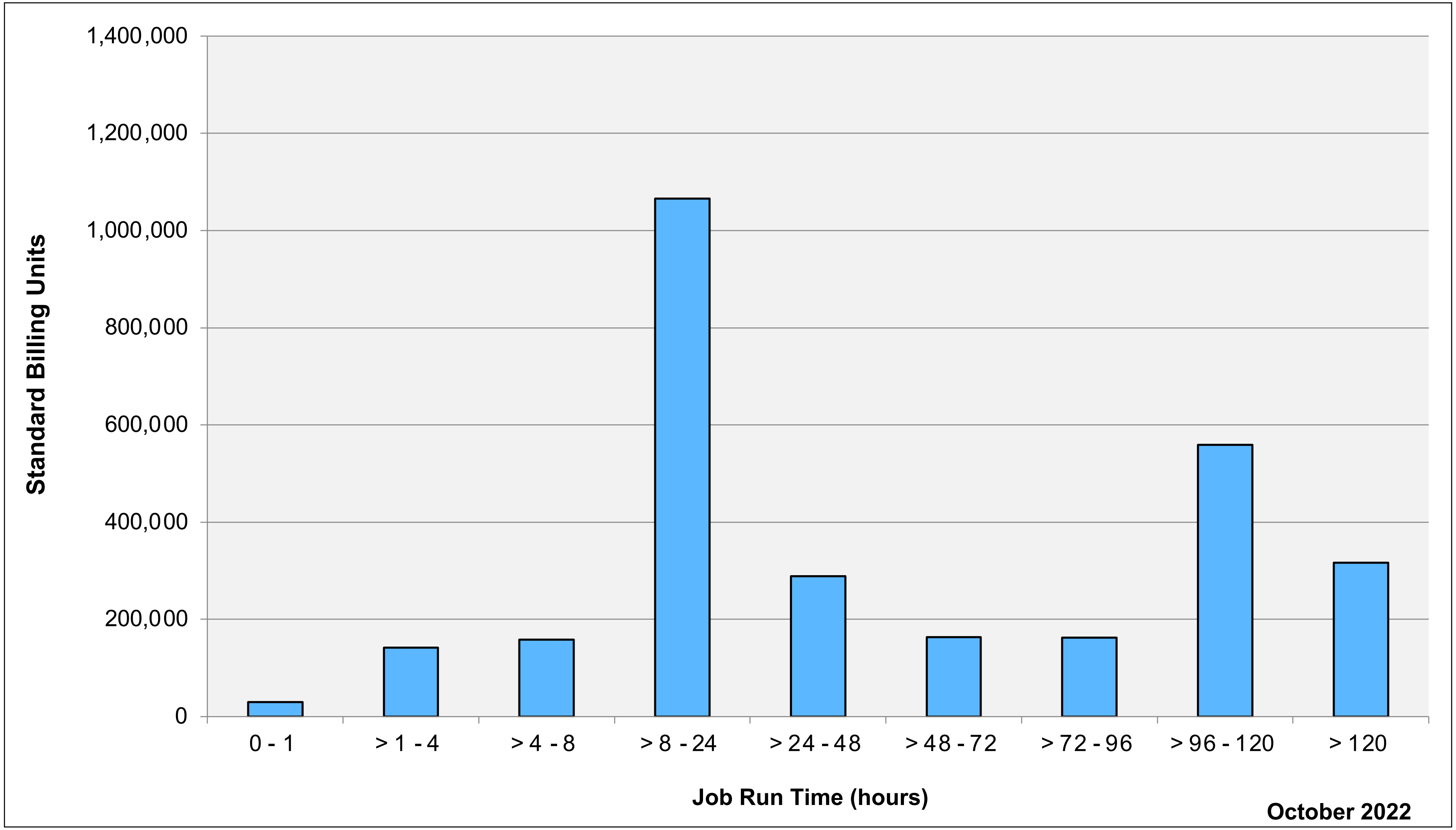
Electra: SBUs Reported, Normalized to 30-Day Month



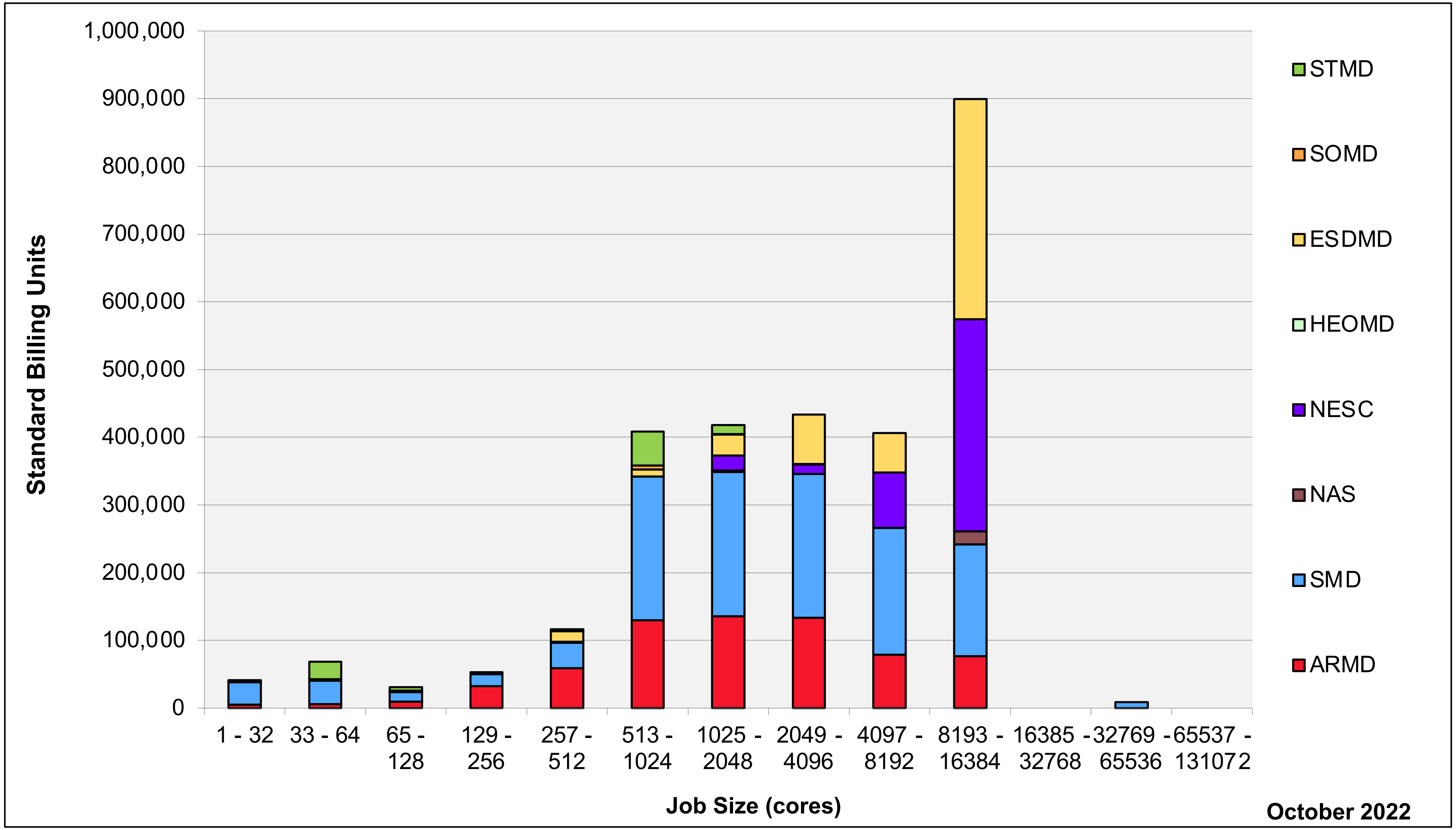
Electra: Devel Queue Utilization



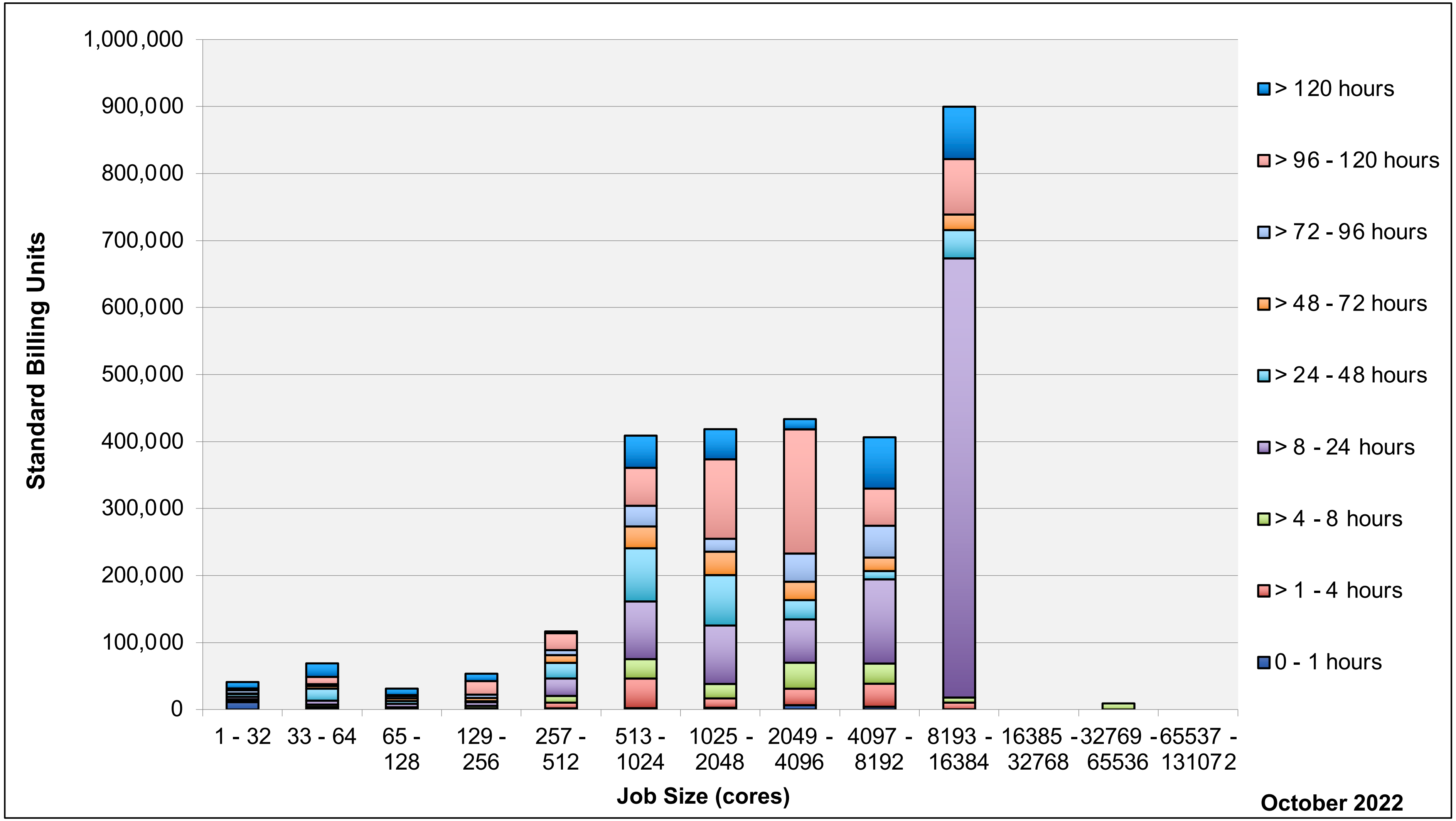
Electra: Monthly Utilization by Job Length



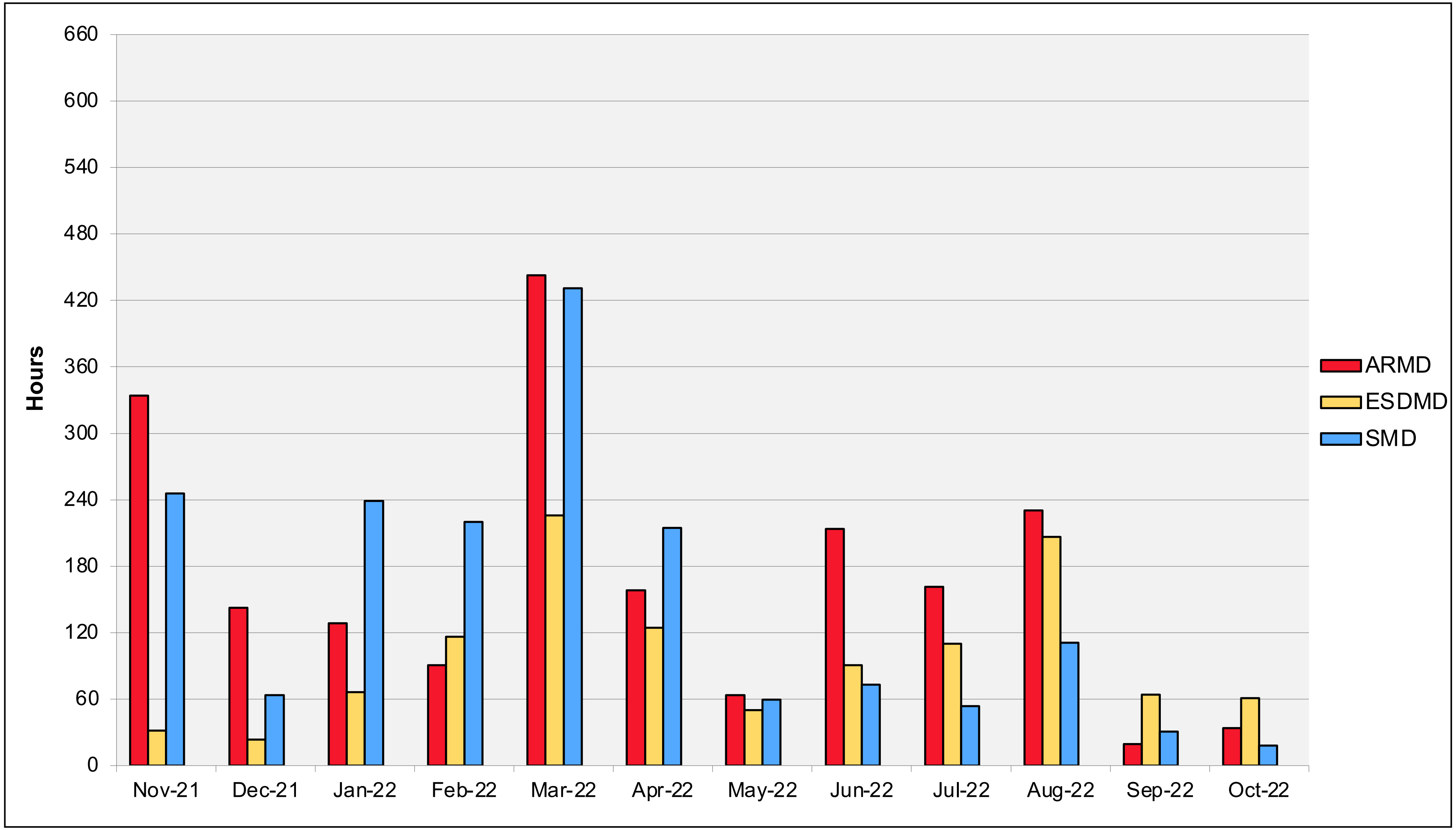
Electra: Monthly Utilization by Job Size



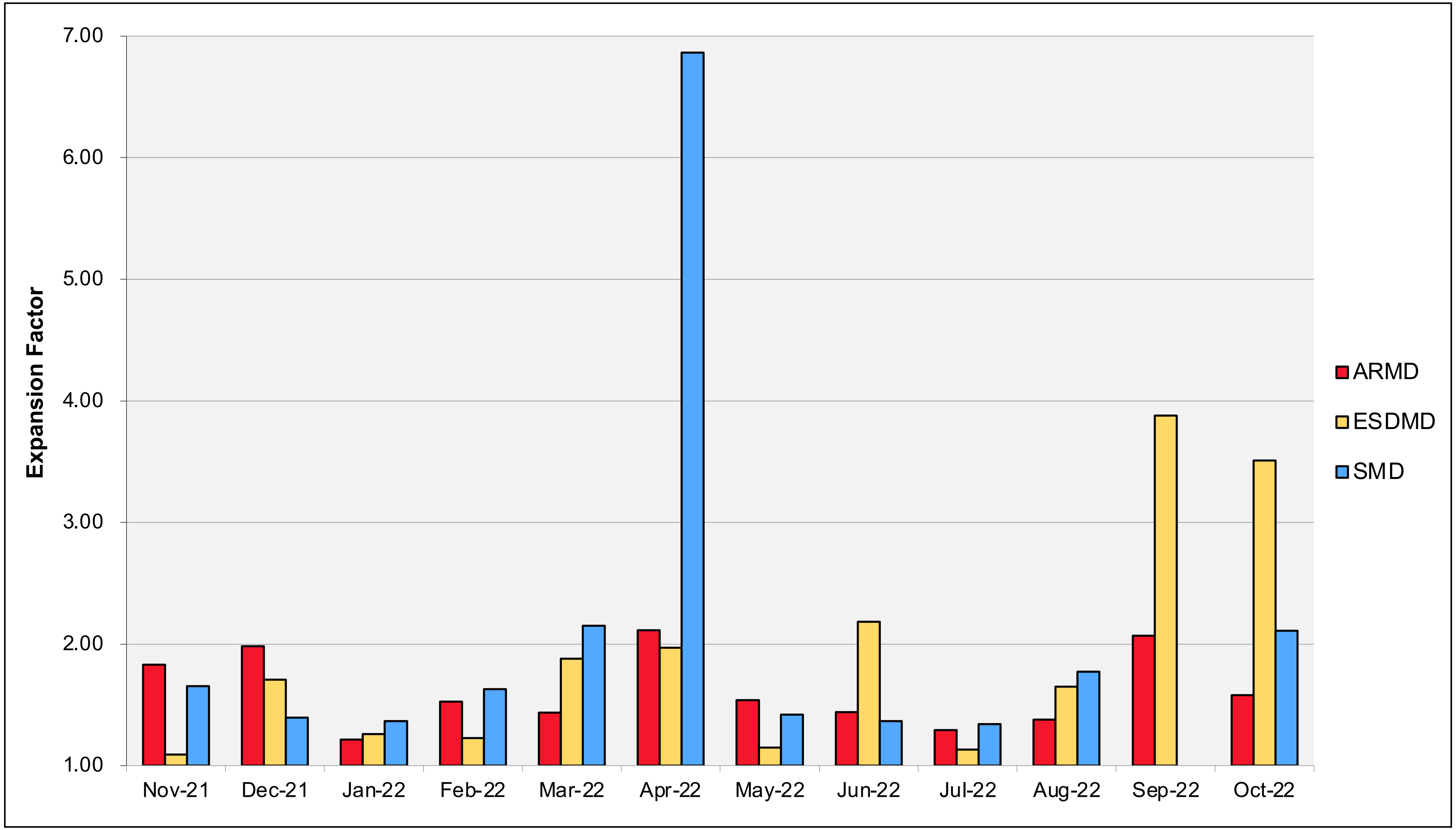
Electra: Monthly Utilization by Size and Length



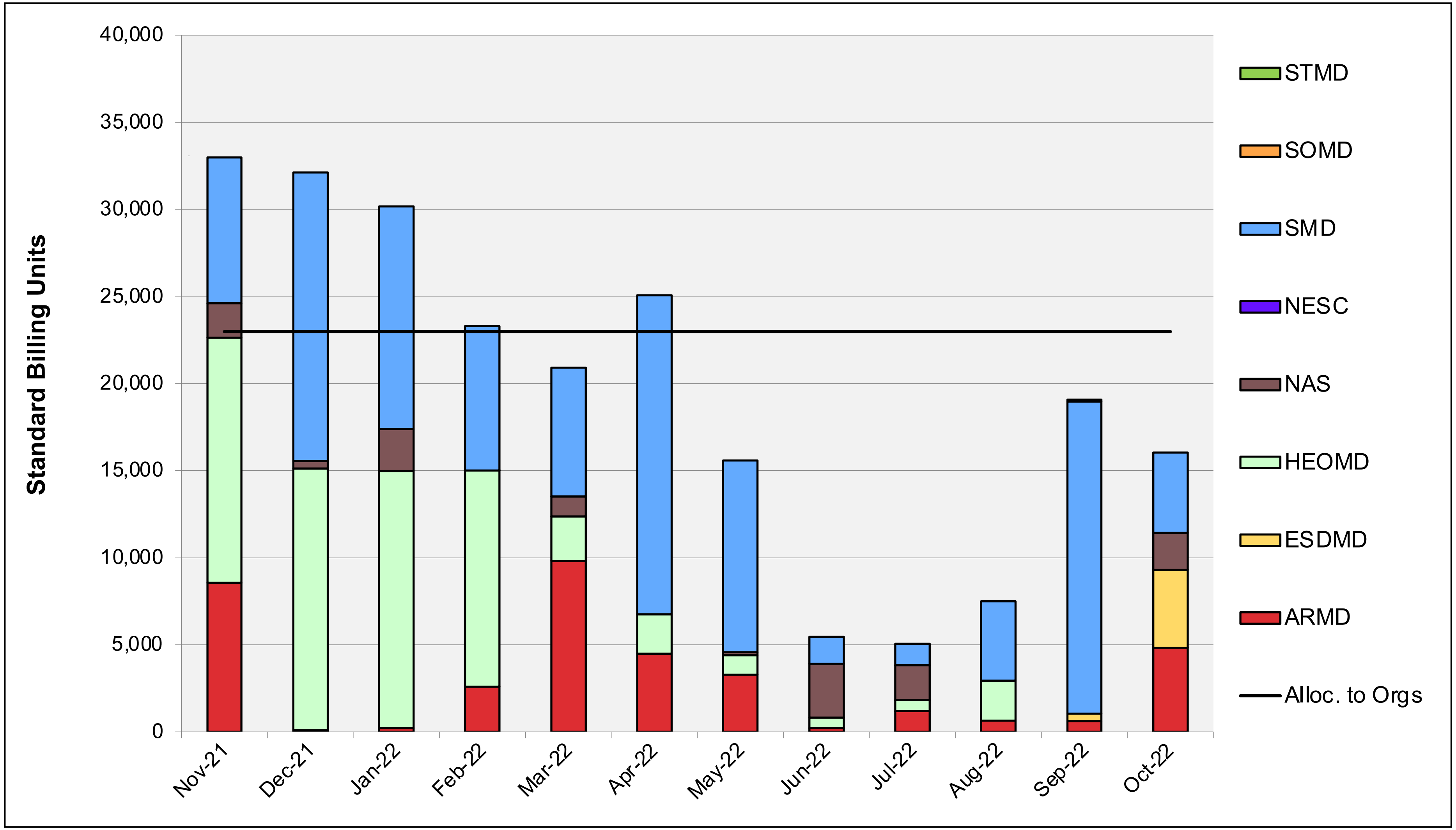
Electra: Average Time to Clear All Jobs



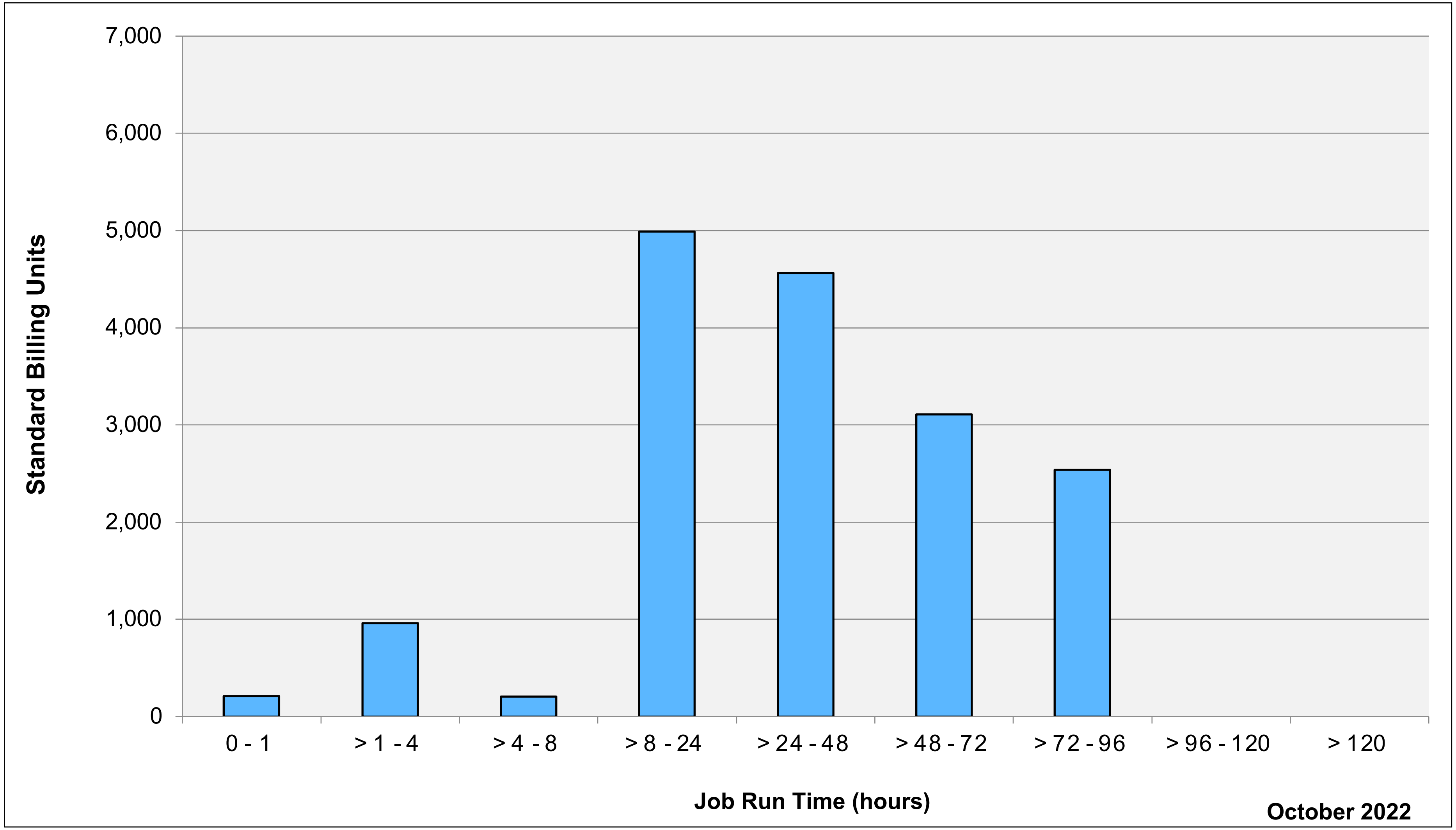
Electra: Average Expansion Factor



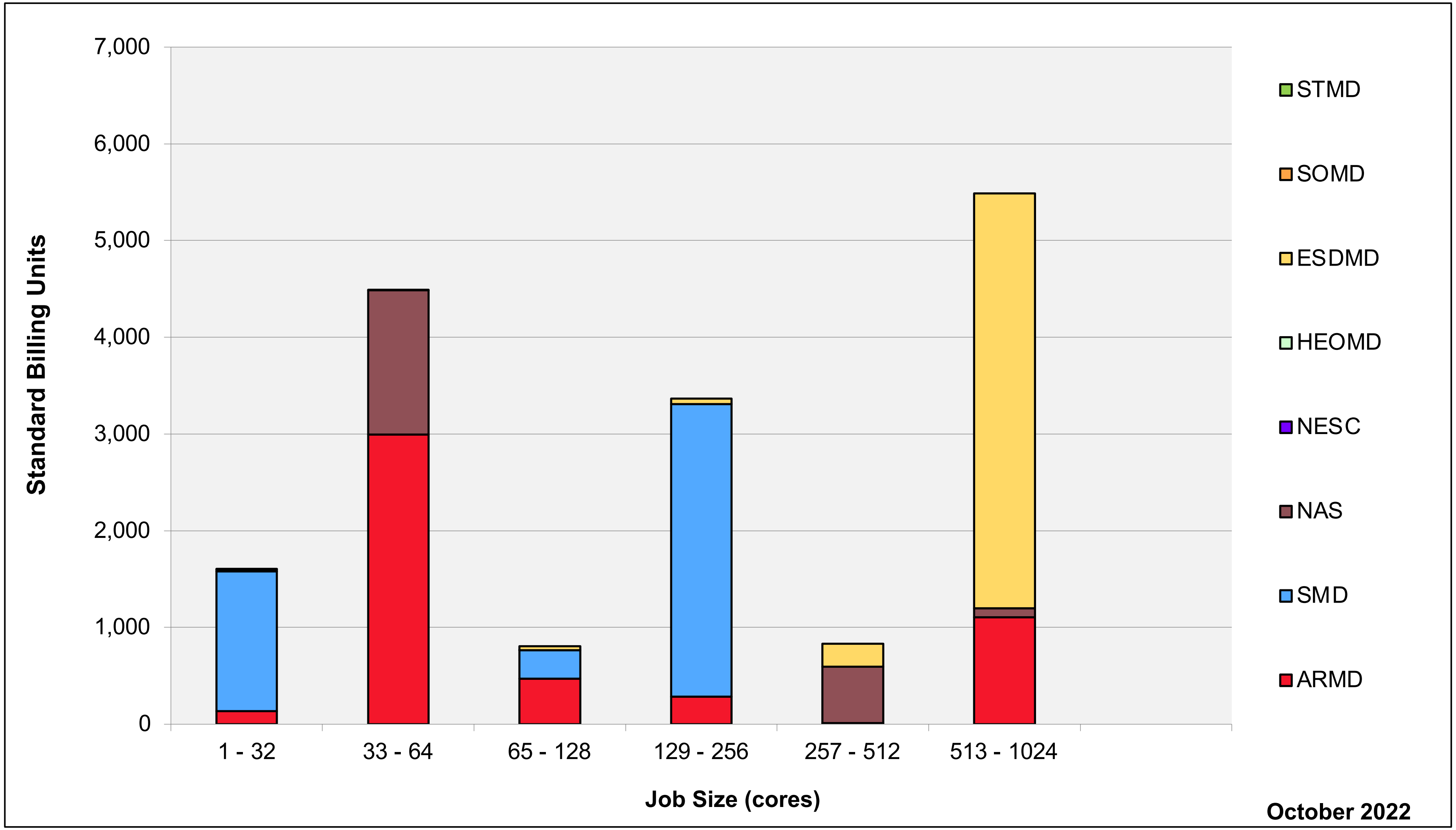
Endeavour: SBUs Reported, Normalized to 30-Day Month



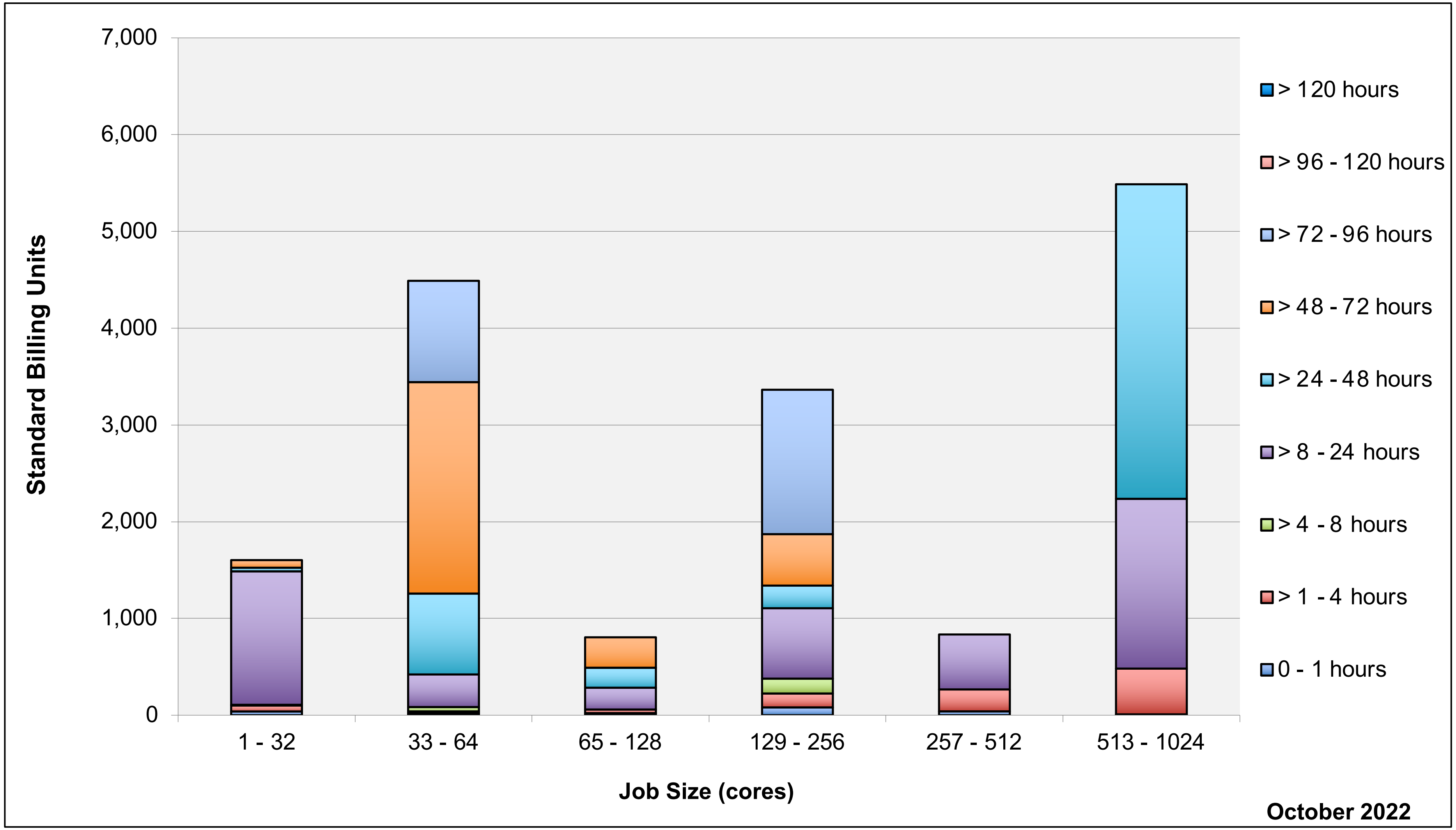
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor